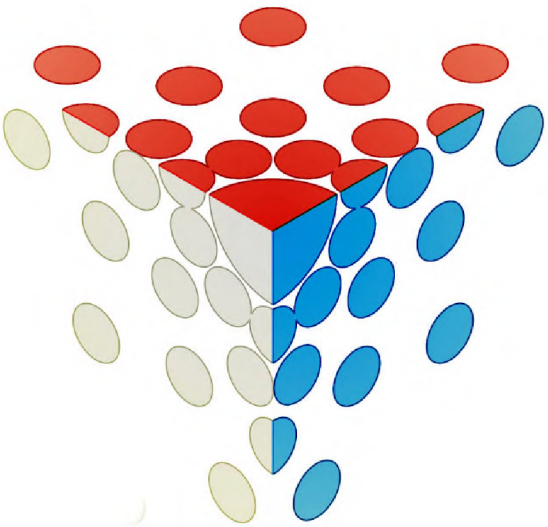
The joint event of

The Eleventh Young Researchers' Conference
Materials Science and Engineering

and

The First European Early Stage Researchers' Conference on
Hydrogen Storage

Belgrade, December 3rd - 5th, 2012



Under the auspices of

Materials Research Society of Serbia
COST Action MP1103
University of Belgrade
Serbian Academy of Sciences and Arts
Italian Embassy

PROGRAM AND THE BOOK OF ABSTRACTS

MATERIALS RESEARCH SOCIETY of SERBIA
INSTITUTE of TECHNICAL SCIENCES of SASA
VINČA INSTITUTE of NUCLEAR SCIENCES, UNIVERSITY of BELGRADE
HYDROGEN STORAGE INITIATIVE SERBIA

PROGRAM AND THE BOOK OF ABSTRACTS

JOINT EVENT OF THE 11TH YOUNG RESEARCHERS' CONFERENCE: MATERIALS SCIENCE AND ENGINEERING

AND

THE 1ST EUROPEAN EARLY STAGE RESEARCHERS' CONFERENCE ON HYDROGEN STORAGE

Edited by:
Jasmina Grbović Novaković
Nenad Ignjatović

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Dear Colleagues,

Welcome to the Joint meeting of **THE ELEVENTH YOUNG RESEARCHERS' CONFERENCE - MATERIALS SCIENCE AND ENGINEERING 2012 & THE FIRST EUROPEAN EARLY STAGE RESEARCHERS' CONFERENCE ON HYDROGEN STORAGE** and the city of Belgrade!

Young Researchers' meetings are held annually late in December since 2002 and they are organized by the Materials Research Society of Serbia. Originally conceived as seminars, since 2007 these meetings were transformed into conferences. The previous ten meetings featured presentations based on the research of various young scientists from Serbia, Bosnia and Herzegovina, Montenegro, Slovenia, Brazil, Germany, United States of America, China, Poland, Belgium, Spain, Romania, United Kingdom, Austria, Italy, Hungary, Russia, Canada, etc. At the Conference, young researchers, students of doctoral, master and undergraduate studies, are given the opportunity to make an overview of their research into materials science and engineering through oral and poster presentations.

As for the scientific content of the conference, we have given full priority to research topics that are currently considered as being on the frontier of the field. Nanotechnology and Advanced Materials, Synthesis and Engineering of Biomaterials, Application of Biomaterials, Theoretical Modeling of Materials and Advanced Methods for Synthesis and Processing present only some of those exciting topics that will be given the central stage and most attention during this meeting. The conference is free of charge and the participants are invited to submit their papers to the journals Tehnika – Novi Materijali, Processing and Application of Ceramics and Energija.

Early Stage Researchers' Conference of Hydrogen Storage is held in Belgrade for the first time under the auspices of the COST ACTION MP 1103. The aim of the meeting is to gather the young researchers from all over Europe and the Word dealing with hydrogen energy, to discuss on the important issues regarding hydrogen storage and production. The papers from this conference will be published in International Journal of Hydrogen Energy Special Issue and Energija in order to disseminate the knowledge and to improve the visibility of our COST Action MP1103.

Prof. Dr. Nenad Ignjatović
Dr. Jasmina Grbović Novaković

MISSION AND GOAL OF COST

COST is an intergovernmental framework for European **Co**operation in **S**cience and **T**echnology, allowing the coordination of nationally-funded research on a European level. As a precursor of advanced multidisciplinary research, COST plays a very important role in building a European Research Area (ERA). It anticipates and complements the activities of the EU Framework Programmes, constituting a "bridge" towards the scientific communities of emerging countries increasing the mobility of researchers across Europe and fostering the establishment of scientific excellence. Through its inclusiveness COST supports integration of research communities, leverages national research investments and addresses issues of global relevance.

One of COST's main characteristics is its flexibility, allowing for an easy implementation and light management of the research initiatives. Activities are launched following a "bottom-up" approach, meaning that the initiative of launching a COST Action comes from the European researchers themselves. The member countries participate on a "à la carte" principle, in that only countries interested in the Action participate.

COST is governed by the COST Member States; 36 COST countries (35 member states and one cooperating state) govern COST. In addition, non-COST country institutions are welcome to participate in the COST programme. COST has also signed reciprocal agreements with Australia, New Zealand, South Africa and Argentina. The organization of COST reflects its intergovernmental nature.

Researchers who wish to launch a new COST Action have to submit a short proposal to the continuous COST Open Call for Proposals, which is then evaluated by the Domain Committee. If the proposal is accepted, the applicants are invited to submit a full proposal with a complete Technical Annex (the scientific and managerial description of an Action). The full proposal is then assessed through a peer review process. Recently, 287 COST Actions are running. Serbia participates in 145 COST Actions.

Prof. Biljana Stojanović, CNC COST Serbia

PROGRAM

of

The 11TH YOUNG RESEARCHERS' CONFERENCE: MATERIALS SCIENCE AND ENGINEERING

Conference program 11YRC

Monday, 3rd December 2012.

8:30- 9:30 Registration

9:30-10:00 Opening ceremony MAIN HALL

Prof. Dr. Nenad Ignjatović, President of the Scientific and Organizing Committee of 11YRC
Prof. Dr. Ivanka Popović, Vice-Rector, University of Belgrade
Prof. Dr. Dragan Uskoković, President of the Materials Research Society of Serbia
Dr. Paolo Battinelli Scientific Attache', Italian Embassy in Belgrade
Prof. Dr. Biljana Stojanović, CNC-COST National Coordinator
Prof. Dr. Amelia Montone, Chair of COST ACTION MP1103
Dr. Jasmina Grbović Novaković, President of the Scientific and Organizing Committee of 1ERS

10:00-10:15 Coffee break

SESSION I Plenary MAIN HALL

Chair: A. Montone, N. Ignjatović

10:15-11:00 **MECANOCHEMISTRY UNDER HYDROGEN GAS: POTENTIALITIES FOR THE SINTHESYS OF EFFICIENT HYDROGEN STORAGE MATERIALS**
Fermin Cuevas, Junxian Zhang, Michel Latroche
Institut de Chimie et des Matériaux Paris-Est, CNRS-UPEC, UMR7182, 2-8 rue Henri Dunant, 94320, Thiais Cedex, France

11:00-11:45 **KEY CONCEPTS IN THE DESIGN OF FUNCTIONAL NANOPARTICLES**
Vuk Uskoković
Therapeutic Micro and Nanotechnology Laboratory, Department of Bioengineering and Therapeutic Sciences, University of California San Francisco, 1700 4th Street, San Francisco, CA 94158-2330, USA

11:45-12:30 **WHAT WE LEARN FROM THE HISTORY TO MASTER THE FUTURE: THE ROLE OF HYDROGEN**
Andreas Züttel
EMPA, Materials Science & Technology, Dübendorf, Switzerland

12:30-14:00 Lunch break

SESSION II Biomaterials Science HALL 16

Chair: Bojana Obradović, Magdalena Stevanović

14:00-14:15 **EFFECTS OF FULLERENOL NANO PARTICLES $C_{60}(OH)_{24}$ ON FILAMENTOUS FUNGUS *ASPERGILLUS NIGER* TIEGH**

Nikola Unković[1], Miloš Stupar[1], Milica Ljaljević Grbić[1], Jelena Vukojević[1], Marina Seke[2], Danica Jović[2], Aleksandar Djordjević[2]

[1]University of Belgrade, Faculty of Biology, Institute of Botany and Botanical Garden "Jevremovac", Takovska 43, 11000 Belgrade, [2]Faculty of Science, Department of Chemistry, Biochemistry and Environment, Trg Dositeja Obradovića 3, 21000 Novi Sad, University of Novi Sad

14:15-14:30 **PHASE AND MICROSTRUCTURAL EVOLUTION DURING SINTERING OF Zr-DOPED HYDROXYAPATITE**

Miodrag J. Lukić[1], Smilja Marković[1], Srečo Davor Škapin[2], Dragan Uskoković[1]

[1]Institute of Technical Sciences of SASA, Belgrade, Serbia, [2]Institute Jozef Stefan, Ljubljana, Slovenia

14:30-14:45 **THE BIOACTIVITY INVESTIGATION OF ELECTRODEPOSITED SILVER/HYDROXYAPATITE/LIGNIN COATINGS IN SIMULATED BODY FLUID**

Sanja Eraković[1], Ana Janković[1], Ivana Matić[2], Zorica Juranić[2], Maja Vukašinović-Sekulić[1], Tatjana Stevanović[3], Vesna Mišković-Stanković[1]

[1]Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia; [2]Institute of Oncology and Radiology of Serbia, University of Belgrade, Belgrade, Serbia; [3]Département des Sciences du Bois et de la Forêt, Université Laval, Québec, Canada

14:45-15:00 **PRODUCTION AND ANTIMICROBIAL ACTIVITY OF FIBERS BASED ON ALGINATE WITH INCORPORATED SILVER NANOPARTICLES**

Srđan Vidović, Milan Stevanović, Maja Vukašinović-Sekulić, Bojana Obradović

Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia

15:00-15:15 **EVALUATION OF NOVEL Ag/ALGINATE MICROBEADS FOR POTENTIAL BIOMEDICAL APPLICATIONS**

Jasmina Stojkovska, Željka Jovanović, Danijela Kostić, Maja Vukašinović-Sekulić, Vesna Mišković-Stanković, Bojana Obradović

Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia,

15:15-15:30 **COPPER – ALGINATE MICROBEADS: BIOACTIVE, ANTIMICROBIAL BIOMATERIALS FOR POTENTIAL BIOMEDICAL APPLICATIONS**

Ivana Madžovska, Maja Vukašinović – Sekulić, Bojana Obradović

Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia

15:30-15:45 **HEMOLYTIC ACTIVITY OF BIOACTIVE NANOCOMPOSITES**

Z. Ajduković[1], N. Ignjatović[2], **N. Petrović[1],** S. Najman[3], J. Rajković[4], D. Kenić Marinković[1], V. Krstić[3], D. Uskoković[2]

[1]University of Niš, Faculty of Medicine, Department of Prosthodontics, Clinic of Stomatology, Niš, Serbia, [2] Institute of Technical Sciencesof SASA, Belgrade, Serbia, [3] University of Niš, Faculty of Medicine, Institute of Biomedical Research, Niš, Serbia, [4] University of Niš, Department of Biology and Ecology, Faculty of Science, Niš, Serbia

15:45-16:00 Coffee break

SESSION II Biomaterials Science HALL 16

Chair: Nebojša Nikolić, Igor Pašti

16:00-16:15 **CHRONOAMPEROMETRIC DETERMINATION OF HYDROGEN-PEROXIDE BY MULTIWALL CARBON NANOTUBES MODIFIED CARBON BASED ELECTRODES**

Jasmina Zbiljić [1], Olga Vajdle [1], Valéria Guzsvány[1], Ákos Kukovecz[2], Zoltán Kónya[2], Božo Dalmacija[1], Kurt Kalcher[3]

[1]University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg D. Obradovića 3, 21000 Novi Sad, R. Serbia, [2]University of Szeged, Department of Applied and Environmental Chemistry, Rerrich 1, 6720 Szeged, Hungary, [3]Karl-Franzens University, Universitätsplatz 3, 8010 Graz, Austria

16:15-16:30 **ELECTROCHEMICAL SYNTHESIS AND CHARACTERIZATION OF SILVER NANOPARTICLES IN POLY(VINYL ALCOHOL) SOLUTION**

Rade Surudžić, Željka Jovanović, Vesna Mišković-Stanković
Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia

16:30-16:45 **VOLTAMMETRIC DETERMINATION OF DOXORUBICIN BY RENEWABLE SILVER-AMALGAM FILM ELECTRODE**

Bojan Tasić, Jasmina Zbiljić, Olga Vajdle, Danica Jović,Valéria Guzsvány, Aleksandar Đorđević
University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg D. Obradovića 3, 21000 Novi Sad, Serbia

16:45-17:00 **CORROSION AND ION RELEASE BEHAVIOR OF NITRIC ACID PASSIVATED STAINLESS STEEL**

Dušan Lj. Petković, Goran M. Radenković
Faculty of Mechanical Engineering, University of Niš, A. Medvedeva 14 Niš, Serbia

17:00-17:15 **VOLTAMMETRIC DETERMINATION OF FENOXANIL FUNGICIDE BY RENEWABLE SILVER-AMALGAM FILM ELECTRODE**

Olga Vajdle[1], Mariola Brycht[2], Jasmina Zbiljić[1],Valéria Guzsvány[1], Sławomira Skrzypek[2]
[1]University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg D. Obradovića 3, 21000 Novi Sad, Serbia, [2]University of Łódź, Department of Instrumental Analysis, Pomorska 163, 90-236, Łódź, Poland

17:15-17:30 **CHARACTERIZATION OF ORGANIC INHIBITOR FOR CORROSION OF MILD STEEL IN 3 WT. % NACL SOLUTION SATURATED WITH CO_2**

Ivana Jevremović[1], Marc Singer[2], Srđan Nešić[2], Vesna Mišković-Stanković[1]
[1]Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia; [2]Institute for Corrosion and Multiphase Technology, Ohio University, Athens, OH, USA

17:30-17:45 **THE INFLUENCE OF ADDITIVES ON THE MORPHOLOGICAL AND CORROSION PROPERTIES OF ELECTRODEPOSITED Zn-Mn ALLOYS**

M. Bučko[1], U. Lačnjevac[2], J. Rogan[1], B. Jokić[1], J.B. Bajat[1]
[1]Faculty of Technology and Metallurgy, University of Belgrade, P.O. Box 3503, 11120 Belgrade, Serbia, [2]Institute for Multidisciplinary Research, University of Belgrade, 11030 Belgrade, P.O. Box 33, Serbia

20-22h Conference dinner HOTEL MOSKVA

Tuesday, 4th December 2012.

8:30-9:00 **Registration**

SESSION IV Synthesis, Characterisation and Properties of Materials Part I
HALL 16

Chair: Smilja Marković, Vladimir Srdić

9:00-9:20 **IDENTIFICATION OF PROMISING CHEMICAL SYSTEMS FOR THE SYNTHESIS OF NEW MATERIALS STRUCTURE TYPES: AN AB INITIO MINIMIZATION DATA MINING APPROACH**

D. Zagorac, J.C. Schön, M. Jansen
Max Planck Institute for Solid State Research, Stuttgart, Germany

9:20-9:35 **KINETICS OF CRYSTALLIZATION OF $Fe_{89.8}Ni_{1.5}Si_{5.2}B_3C_{0.5}$ AMORPHOUS ALLOY**

Milica M. Vasić[1], Vladimir A. Blagojević[1], Dušan M. Minić[2], Dragica M.Minić[1]
[1]Faculty of Physical Chemistry, University of Belgrade, Serbia
[2]Military Technical Institute, Belgrade, Serbia

9:35-9:50 **CHARACTERIZATION OF PULSED LASER DEPOSITED CDS ON TiO_2 NANOTUBES ARRAYS**

A. Bjelajac[1], V. Djokić[1], R. Petrović[1], G. Socol[2], I. Mihailescu[2], I. Florea[3], O. Ersen[3], Dj. Janaćković[1]
[1]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia, [2]National Institute for Lasers, Plasma, and Radiation Physics, Bucharest-Magurele, Romania, [3]Institut de Physique et Chimie des Materiaux de Strasbourg, CNRS - Universite de Strasbourg (UDS) UMR 7504, 23, rue du Loess, BP 43, 67037 Strasbourg cedex 02, France

9:50-10:05 **INFLUENCE OF PARTICLE SIZE AND MORPHOLOGY OF ZNO POWDERS ON THEIR OPTICAL PROPERTIES**

A. Stanković[1], Z. Stojanović[1], Lj. Veselinović[1], N. Abazović[2], S.D. Škapin[3], S. Marković[1], D. Uskoković[1]

[1]Institute of Technical Sciences of SASA, Belgrade, Serbia, [2]Vinča Institute of Nuclear Science , Belgrade, Serbia, [3]Jožef Štefan Institute, Ljubljana, Slovenia,

10:05-10:20 **COMPACTION PRESSURE'S INFLUENCE ON DENSITY AND ELECTRICAL PROPERTIES OF SINTERED CORDIERITE-BASED CERAMICS**

N. Obradović[1], N. Đorđević[2], **A. Peleš[1]**, M. Mitrić[3], V. Pavlović[1]

[1]Institute of Technical Sciences of SASA, Knez Mihajlova 35/IV, 11000 Belgrade, Serbia, [2]Institute for Technology of Nuclear and Other Mineral Raw Materials, Bulevar Franse d'Eperea 86, 11000 Belgrade, Serbia, [3]Vinča institute of Nuclear Sciences, University of Belgrade, Mike Alasa 12-14, 11000 Belgrade, Serbia

10:20-10:35 **DEPOSITION OF THE DLC STRUCTURES IN THE LOW-PRESSURE OXY-ACETYLENE FLAT FLAME**

Bojana Radojković[1], Marija Krmar[1], Miroljub Vilotijević[2], Bojan Gligorijević[1], Ana Alil[1]

[1]Institute Goša, Milana Rakića 35, Belgrade, Serbia, [2]University of Belgrade, Vinča Institute of Nuclear Sciences "", 11001 Belgrade, Serbia

10:35-10:50 **CHEMICAL STABILITY OF $Fe_x(Sb_2S_3)_{0.75}(SbI_3)_{0.25})_{1-x}$ GLASSES**

N. Ćelić, **M. D. Vučkovac**, I. O. Gut, M. Avramov

University of Novi Sad, Faculty of Sciences, Department of Physics, Trg D. Obradovića 4, Novi Sad, Serbia

10:50-11:10 Coffee break

SESSION V Theoretical Modelling of Materials HALL 16

Chair: Željka Nikitović, Nebojša Mitrović

11:10-11:25 **WELDING PARAMETERS PREDICTION BY THE ANALYTICAL METHODS AND USE OF NUMERICAL SIMULATION SOFTWARE FOR GS-36MN5 STEEL**

S. Budimir, B. Jegdić, **M. Prokolab**, M. Prvulović, Z. Milutinović
Institut Goša, Milana Rakića 35, Beograd, Srbija

11:25-11:40 **CALCULATION OF TEMPERATURE DISTRIBUTION OF THE POWDER PARTICLES IN THE SPRAY DEPOSITION PROCESS**

Milorad Kočić, **Mirjana Prvulović**, Jasmina Obradović, Marko Ristić, Milan Prokolab
Institute Goša, Milana Rakića 35, 11000 Belgrade, Serbia

11:40-11:55 **APPLICATION OF FINITE ELEMENTS METHOD IN ANALYSIS OF DYNAMIC BEHAVIOR OF COMPOSITE LAMINATES**

Dragan Čukanović[1], Aleksandar Radaković[2], Miroslav Živković[3]
[1]Faculty of Technical Sciences, Kosovska Mitrovica, [2]State University in Novi Pazar, [3]Faculty of Engineering, Kragujevac, Serbia

11:55-12:15 **PROPAGATION OF BULK WAVES IN A TRANSVERSAL ISOTROPIC MEDIUM**

Radaković Aleksandar[1], Čukanović Dragan[2], Dragan Milosavljević[3], Gordana Bogdanović[3], Ljiljana Veljović[3]
[1]State University in Novi Pazar, [2]Faculty of Technical Sciences, Kosovska Mitrovica, [3]Faculty of Engineering, Kragujevac, Serbia

12:15-12:30 **ON THE TRANSITION FROM DELOCALIZED TO LOCALIZED VIBRON STATES IN MACROMOLECULAR CHAINS**

M. Nešić, S. Galović, D. Čevizović
Vinča Institute of Nuclear Sciences, University of Belgrade, Serbia

12:30-12:45 **SUBSTITUTION EFFECTS OF SUMANENE BENZYLIC POSITIONS WITH BORON AND NITROGEN ATOMS**

Stevan Armaković[1], Sanja J. Armaković[2], Igor J. Šetrajčić[1], Jovan P. Šetrajčić[1,*]
[1]University of Novi Sad, Faculty of Sciences, Department of Physics, Trg Dositeja Obradovića 4, 21000, Novi Sad, Vojvodina, Serbia, [2]University of

Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000, Novi Sad, Vojvodina, Serbia, *Academy of Sciences and Arts of Republic of Srpska, Bana Lazarevića 1, 78000 Banja Luka, Republic of Srpska, B&H

12:45-13:00 **THERMAL PROPERTIES OF CARBON NANOTUBES**

Z. P. Popović, M. Damnjanović, I. Milošević
NanoLab, Faculty of Physics, University of Belgrade, Serbia

13:00- 13:15 **NEWS FROM JEOL - ELECTRON MICROSCOPES AND SPECTROMETERS –** Slavko Žižek, univ.dipl.inž.el.,Scan d.o.o **HALL 16**

13:15-14:00 Lunch break

SESSION VI Synthesis, Characterisation and Properties of Materials Part II
HALL 16

Chair: Dragana Jugović, Vladimir Srdić

14:00-14:20 **RAMAN SCATTERING STUDY OF IRON-CHALCOGENIDE SUPERCONDUCTORS**

N. Lazarević[1], S. Bogdanović[1], Hechang Lei[2], C. Petrović[2], Z. V. Popović[1]
[1]Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia, [2]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973-5000, USA

14:20-14:35 **EFFECTS OF OPTICAL BEAM MULTIPLE REFLECTIONS TO PHOTOTHERMAL RESPONSE - CORRECTION FACTOR**

Slobodan Todosijević[1], Zlatan Šoškić[1], Nebojša Bogojević[1], Dalibor Čevizović[2], Slobodanka Galović[1,2,3]
[1]Faculty of Mech. Eng. Kraljevo, University of Kragujevac, Dositejeva 19, Kraljevo, Serbia, [2]Vinča Institute of Nuclear Sciences, University of Belgrade, p.o.Box 522, Belgrade, Serbia, [3]Joint Institute for Nuclear Research, Bogoliubov Laboratory of Theoretical Physics, Dubna, Russia

14:35-14:50 **SiC MOSFET – MODEL OF CURRENT-VOLTAGE CHARACTERISTICS AND POSSIBILITIES FOR IT'S IMPLEMENTATION IN BIOMEDICAL ELECTRO EQUIPMENT**

Zorana Z. Golubović[1], Petar M. Lukić [1], Milan T. Milovanović[2], Vladan M. Lukić[1], Rajko M. Šašić[3]
[1]Faculty of Mechanical Engineering, University of Belgrade, Kraljice Marije 16, 11120 Belgrade, Serbia, [2]Military Medical Academy, Crnotravska 17, 11000 Belgrade, Serbia, [3]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade

14:50-15:05 **STUDY OF THE SHUNGITE AND COANP STRUCTURES NONLINEAR PROPERTIES**

Svetlana Likhomanova, Natalia V. Kamanina
Vavilov State Optical Institute, 12, Birzhevaya Line, St.-Petersburg, 199034, Russia

15:05-15:20 **STUDY OF THE CARBON NANOTUBES INFLUENCE ON THE REFLECTION SPECTRUM AND THE MICROHARDNESS OF KBr, BaF_2**

Pavel V. Kuzhakov, Natalia V. Kamanina
Vavilov State Optical Institute, 12, Birzhevaya Line, St.-Petersburg, 199034, Russia

15:20-15:35 **TG-DTG STUDY OF BULK As_2S_3 CHALCOGENIDE GLASSES DOPED WITH BISMUTH**

M. R. Dimitrievska, M. Šeljegović, Lj. Dačanin, K. Čajko
University of Novi Sad, Department of Physics, Trg Dositeja Obradovića 4, Novi Sad, Serbia

15:35-15:50 **SYNTHESIS AND CHARACTERIZATION OF $NiFe_2O_4/BaTiO_3$ THIN FILMS**

Branimir Bajac[1,*], Jelena Vukmirović[1], Ivan Tokić[1], Stevan M. Ognjanović[1], Akos Kukovecz[2], Vladimir V. Srdić[1]
[1]Department of Materials Engineering, Faculty of Technology, University of Novi Sad, Novi Sad, Serbia, [2]Department of Applied and Environmental Chemistry, University of Szeged, Szeged, Hungary

15:50-16:05 **PHASE DIAGRAM OF SYSTEM $ZnGeAs_2$-$CdGeAs_2$**

I.V. Fedorchenko[1], A.N. Aronov[1], A.H. Yusupov[2], L. Kilanski[3], V. Domuchowski[3]
[1]Kurnakov Institute of General and Inorganic Chemistry Russain Academy of Sciences, 119991, Moscow, Russia, Leninskiy pr.31,

[2]National University of Science and Technology"MISIS",119049, Moscow, Russia, Leninskiy pr.4, [3]Institute of physics, Polish Academy of Sciences, 02-668, Warsaw, Poland, al. Lotnikow 32/46

16:15 -18:00 **POSTER SESSION** and coffee break

SASA Gallery of Science and Technology, Đure Jakšića 2

Chair: Bojana Obradović, Željka Nikitović, Smilja Marković

Wednesday, 5th December 2012.

9:00-9:30 **Registration**

SESSION VII Polymeric Materials HALL 16

Chair: Gordana Ćirić-Marjanović, Edin Suljovrujić

9:30-9:45 **THE INFLUENCE OF THE STRUCTURE OF THE POLYBUTADIENE BLOCK TO THE MECHANICAL PROPERTIES OF THE POLYSTYRENE-b-POLYBUTADIENE-b-POLY(METHYL METHACRYLATE) COPOLYMER**

Dragutin Nedeljković, Aleksandar Stajčić, Aleksandar Grujić, Jasmina Stevanović, Jasna Stajić-Trosić
University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Njegoševa 12, Belgrade, Serbia

9:45-10:00 **INFLUENCE OF GOLD IONS IMPLANTATION AND OZONE TREATMENT ON SURFACE CHARACTERISTICS OF HIGH DENSITY POLYETHYLENE**

Danilo Kisić[1], Miloš Nenadović[1], Borivoj Adnađević[2], Zlatko Rakočević[1]
[1]INS Vinča, Laboratory of Atomic Physics, University of Belgrade, Mike Alasa 12–14, 11001 Belgrade, Serbia, [2]Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, 11158 Belgrade, Serbia

10:00-10:15 **SURFACE DIELECTRIC PROPERTIES AND FOURIER TRANSFORM INFRARED (FTIR) SPECTROSCOPY SPECTRA OF LOW-DENSITY POLYETHYLENE (LDPE) ETCHED BY TRICHLOROACETIC ACID AT DIFFERENT TEMPERATURES**

K. Simonović[1], F. Marinković[1], J. Dojčilović[1], D. Dudić[2]
[1]Faculty of Physics, University of Belgrade, Studentski trg 12-16, 11001 Belgrade, Serbia, [2]Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

10:15-10:30 **NOVEL ASYMMETRIC POLYETHERSULFONE MEMBRANES FOR ULTRAFILTRATION APPLICATION**

Aleksandra Nešić[1], Sava Veličković[2], Filip Radovanović[3], Aleksandra Nastasović[3]

[1]VinčaInstitute for Nuclear Sciences , University of Belgrade, Mike Petrovića Alasa 12-14, Belgrade, Serbia, [2]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia, [3]Institute for Chemistry, Technology and Metallurgy, University of Belgrade, Studentski trg 16, Belgrade, Serbia

10:30-10:45 **SURFACE MODIFICATION OF PECTIN SPHERES CROSS-LINKED IN LEAD(IV) AND COPPER(II) SOLUTIONS**

Sanja Šešlija[1], Jasmina Stevanović[2], Tatjana Volkov-Husović[3], Sava Veličković[3]

[1]Innovation Centre of the Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, [2]Institute of Chemistry, Technology and Metallurgy, Department of Electrochemistry, Belgrade, Serbia, [3]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

10:45-11:00 Coffee break

SESSION VII Polymeric Materials HALL 16

Chair: Gordana Ćirić-Marjanović, Edin Suljovrujić

11:00-11:15 **FERROMAGNETIC POLYANILINE/TiO_2 NANOCOMPOSITES**

Marija Radoičić[1], Zoran Šaponjić[1], Gordana Ćirić–Marjanović[2], Zorica Konstantinović[3], Jovan Nedeljković[1]

[1]Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, [2]Faculty of Physical Chemistry, University of Belgrade, Belgrade 11158, Serbia, [3]Institut de Ciéncia de Materials de Barcelona, CSIC, Bellaterra 08193, Spain

11:15-11:30 **COMPARISON OF DIELECTRIC PROPERTIES OF POLYVINYLIDENE FLUORIDE + Cu COMPOSITES MEASURED BY SINUSOIDAL AND TRIANGLE SIGNALS**

I. Petronijević[1], K. Simonović[1], R. Dojčilović[2] V. Đoković[2], D. Dudić[2]

[1]Faculty of Physics, University of Belgrade, Studentski trg 12-16, 11001 Belgrade, Serbia, [2] Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

11:30-11:45 **POLY(METHACRYLIC ACID)/ZEOLITE HYDROGEL COMPOSITES AS ADSORBENTS FOR CATIONIC DYE REMOVAL**

Vesna V. Panić[1], Željka Madžarević[2], Tatjana Volkov-Husović[2], Sava J. Veličković[2]

[1]Innovation Center of Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia, [2]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia

11:45-12:00 **SYNTHESIS OF POLYSTYRENE-*G*-STARCH COPOLYMERS USING NEW INITIATOR/*CO*-INITIATOR SYSTEM**

Vladimir Nikolić[1], Veličković Sava[2], Popović Aleksandar[3]

[1]Innovation Center, Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, 11000 Belgrade, Serbia, [2]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia, [3]Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, 11000 Belgrade, Serbia

12:00-12:15 **A SURVEY OF GRP PIPES DEFECTS AND DAMAGE DUE TO FABRICATION PROCESSES**

Abdelrhaman Aljadeed[1], Ahamed Younaes[1], Ramadan A. Al-Madani[1], M. Jarnaz[2]

[1]Al-Jabel Algharbi University, Engineering Faculty, Gharian, Libya, [2]Academy of Graduate Studies, Tripoli - Libya

12:15-12:30 Awards and closing ceremony

POSTER SESSION 11YRC SASA Gallery of Science and Technology (Đure Jakšića 2)

NOTE: Please bring the posters to the conference registration desk on 03.12.2012

Y1. INVESTIGATION OF THE STRUCTURE OF NANOSIZED Na_nCl_n (n = 8, 16, 24, 32) CLUSTERS USING GLOBAL OPTIMIZATION

J. Zagorac[1,2], J. C. Schön[1], M. Jansen[1]

[1]Max Planck Institute for Solid State Research, Stuttgart, Germany, [2]Materials Science Laboratory, Vinča Institute of Nuclear Sciences , Serbia

Y2. ELECTRICAL PROPERTIES OF MULTIDOPED CERIA

M. Stojmenović[1], B. Matović[1], M. Žunić[2]

[1]Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, [2]Institute for Multidisciplinary Research, University of Belgrade, Belgrade, Serbia

Y3. DOPED WITH Cu AND Mn ZINC OXIDE CATALYSTS FOR OXIDATION OF CO IN NOXIOUS EMISSIONS

Katya Milenova[1], Penko Nikolov[2]

[1]Institute of Catalysis, Bulgarian Academy of Sciences, Akad. G. Bontchev str. bl 11, 1113, Sofia, Bulgaria, [2]University of Chemical Technology and Metallurgy, 8 Kliment Ohridski, 1756, Sofia, Bulgaria

Y4. MINIMAL REQUIRED WALL THICKNESS COMPARATIVE ANALYSIS OF A STABLE TANK MADE OF STAINLESS STEEL WITH AND WITHOUT STRAIN HARDENING

Katarina Jovičić[1], Iva Najvirt[2], Ana Alil[1], Milica Pilipović[3]

[1]Institut Goša d.o.o., Milana Rakića 35, 11000 Belgrade, Serbia, [2]Nordvik d.o.o., Pariske Komune 22, 11000 Belgrade, Serbia, [3]Grundfos Srbija d.o.o., Omladinskih Brigada 90b, 11000 Belgrade, Serbia

Y5. REDUCING THE PARTICLE SIZE OF Bi_20_3 AND Fe_20_3 FOR THE SYNTHESIS OF $BiFeO_3$

Maria Čebela, Marija Prekajski, Mia Omerašević, Branko Matović

Materials Science Laboratory, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

Y6. COMPARATIVE ANALYSIS OF CESIUM SORPTION BEHAVIOR OF THERMALLY, MECHANO-CHEMICALLY MODIFIED AND RAW DIATOMITE

Mia O. Omerašević[1], Miljana M. Mirković[1], Uroš D. Jovanović[2], Anja Došen[1], Ljijana M. Kljajević[1], Maria Ž. Čebela[1], Snežana S. Nenadović[1]

[1]Laboratory for Material Science, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, [2]Laboratory of Chemical Dynamics and Permanent Education, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

Y7. ELECTRON SPIN RESONANCE STUDY OF GAMMA-IRRADIATED PLLA

D. Miličević, D. Milivojević, E. Suljovrujić
Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

Y8. ADSORPTION OF ARSENIC(III) FROM AQUEOUS SOLUTIONS ON CARBON CRYOGEL

Tamara Minović, Biljana Babić, Milovan Stoiljković, Vesna Maksimović, Jelena Gulicovski, Jelena Pantić, Branko Matović
Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

Y9. THE EFFECT OF CHEMICAL COMPOSITION ON SWELLING AND MECHANICAL PROPERTIES OF P(HEMA/IA/OEGA) HYDROGELS

M. Mićić, E. Suljovrujić
Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

Y10. NUMERICAL SIMULATION OF ROPEWAY OF AIRLIFT VEHICLES: CALCULATION METHODS

Miranda Kullolli, **Alfred Hasanaj**
Polytechnic University of Tirana, Albania

Y11. LOCAL AND ELECTRONIC STRUCTURE AROUND MANGANESE IN MULTI-COMPONENT SEMICONDUCTORS

M. Medić, I. Radisavljević, N. Novaković, B. Kuzmanović, B. Paskaš Mamula, N. Ivanović
Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

Y12. SURFACE DIELECTRIC RELAXATIONS OF ISOTACTIC POLYPROPYLENE (iPP) AFTER ILLUMINATION AT DIFFERENT TEMPERATURES

V. Čubrović[1], I. Petronijević[1], J. Dojčilović[1], D. Dudić[2]
[1]Faculty of Physics, University of Belgrade, Studentski trg 12-16, 11001 Belgrade, Serbia
[2]Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

Y13. SURFACE DIELECTRIC PROPERTIES OF LOW-DENSITY POLYETHYLENE (LDPE) IN VARIABLE VISIBLE LIGHT CONDITIONS

F. Marinković[1], V. Čubrović[1], J. Dojčilović[1], D. Dudić[2]
[1]Faculty of Physics, University of Belgrade, Studentski trg 12-16, 11001 Belgrade, Serbia, [2] Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

Y14. NEW FACILE SYNTHESIS ROUTE FOR OBTAINING PHASE PURE $LiFePO_4$/C COMPOSITE

M. Milović[1], D. Jugović[1], M. Mitrić[2], B. Jokić[3], D. Uskoković[1]

[1]Institute of Technical Sciences of SASA, Belgrade, Serbia, [2]Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, [3]Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

Y15. BIOACTIVE COMPOSITE MATERIALS IN REGENERATION OF THE RESORBED BONE OF ALVEOLAR RIDGES

Z. Ajduković[1], N. Ignjatović[2], **J. Rajković[3],** S. Najman[4], D. Mihailović[5], N. Petrović[1], D. Kenić Marinković[1], D. Uskoković[2]

[1]Department of Prosthodontics, Clinic of Stomatology, Faculty of Medicine University of Niš, Serbia, [2]Institute of Technical Sciences of SASA , Belgrade, Serbia, [3]Department of Biology and Ecology, Faculty of Science and Mathematics, University of Niš, Serbia, [4]Institute for Biomedical Research, Faculty of Medicine, University of Niš, Serbia, [5] Institute of Pathology, Faculty of Medicine, University of Niš, Serbia

Y16. EFFECTS OF DIFFERENT CRYOPROTECTANTS ON MORPHOLOGY OF LYOPHILIZED POLY(E-CAPROLACTONE) MICRO- AND NANOSPHERES

Petar Stupar[1], Magdalena Stevanović[2], Nenad Filipović[2], Vladimir Pavlović[2,3], Jana Nunić[4], Sandra Cundrič[5], Metka Filipič[4], Dragan Uskoković[2]

[1]Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, [2]Institute of Technical Sciences of , Belgrade, Serbia, [3]Faculty of Agriculture, University of Belgrade, Belgrade, Serbia, [4]Department of Genetic Toxicology and Cancer Biology, National Institute of Biology, Ljubljana, Slovenia, [5]Biotechnical Faculty, University of Ljubljana, Ljubljana, Slovenia

Y17. SYNTHESIS AND CHARACTERIZATION OF SELENIUM NANOPARTICLES IN THE PRESENCE OF BOVINE SERUM ALBUMIN OR POLY (L-GLUTAMIC ACID) FOR BIOMEDICAL APPLICATION

Nenad Filipović[1], Magdalena Stevanović[1], Srečo D. Škapin[2], Ines Bračko[2], Dragan P. Uskoković[1]

[1]Institute of Technical Sciences of SASA, Knez Mihailova 35/IV, 11000 Belgrade, Serbia, [2]Advanced Materials Department, Jožef Štefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

Y18. THE EFFECT OF AGING OF MILLED CLAY ON THE REMOVAL EFFICIENCIES OF HEAVY METAL IONS

Anđelka Đukić[1], Ksenija Kumrić[2], Tatjana Trtić-Petrović[2], Jasmina Grbović Novaković[1], Sanja Milošević[1], Igor Milanović[1], Ljiljana Matović[1]

[1]Laboratory of Materials Sciences, Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia, [2]Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

Y19. DRUG DELIVERY PARADIGM OF SILVER IONS RELEASED FROM AG/PVA HYDROGEL NANOCOMPOSITES OBTAINED BY RADIATION CHEMISTRY NANOREACTOR METHOD

Jelena Krstić, Jelena Spasojević, Aleksandra Radosavljević, Zorica Kačarević-Popović
Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

Y20. SWELLING STUDIES OF THERMO- AND pH-SENSITIVE Ag-POLY(NiPAAm/IA) HYDROGEL NANOCOMPOSITES SYNTHESIZED BY GAMMA IRRADIATION

Jelena Spasojević[1], Jelena Krstić[1], Aleksandra Radosavljević[1], Melina Kalagasidis-Krušić[2], Zorica Kačarević-Popović[1]
[1]Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, [2]Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

Y21. KINETIC STUDY OF PALLADIUM SORPTION BY MACROPOROUS COPOLYMER

Bojana Ekmeščić[1], Danijela Maksin[2], Jelena Marković[2] Aleksandra Nastasović[1] Antonije Onjia[2]
[1]University of Belgrade, Institute for Chemistry, Technology and Metallurgy, Njegoševa 12, Belgrade, Serbia, [2]University of Belgrade, Vinča Institute of Nuclear Sciences, Mike Petrovića Alasa 12-14, Vinča, Serbia

Y22. EXAMINATION OF THE INFLUENCE OF NANOMATERIALS CALCIUM PHOSPHATE/POLY-(DL-LACTIDE-CO-GLYCOLIDE) AND COBALT-EXCHANGED HYDROXYAPATITE ON THE VIABILITY OF SAOS-2 CELLS

Stevo Najman[1], **Sanja Stojanović**[1], Žarko Mitić[2], Zorica Ajduković[3], Nenad Ignjatović[4], Dragan Uskoković[4]
[1]University of Niš, Faculty of Medicine, Institute of Biology and Human Genetics, Serbia ,[2]University of Niš, Faculty of Medicine, Department of Pharmacy, Serbia, [3]University of Niš, Faculty of Medicine, Clinic of Stomatology, Department of Prosthodontics, Niš, Serbia,[4]Institute of Technical Sciences of SASA, Belgrade, Serbia

PROGRAM

of

The 1st EUROPEAN EARLY STAGE RESEARCHERS' CONFERENCE
on HYDROGEN STORAGE
COST MP1103

Conference program 1EESRC

Monday, 3rd December 2012.

8:30-9:30 Registration

9:30-10:00 Opening ceremony MAIN HALL

Prof. Dr. Nenad Ignjatović, President of the Scientific and Organizing Committee of 11YRC
Prof. Dr. Ivanka Popović, Vice-Rector, University of Belgrade
Prof. Dr. Dragan Uskoković, President of the Materials Research Society of Serbia
Dr. Paolo Battinelli Scientific Attache', Italian Embassy in Belgrade
Prof. Dr. Biljana Stojanović, CNC-COST National Coordinator
Prof. Dr. Amelia Montone, Chair of COST ACTION MP1103
Dr. Jasmina Grbović Novaković, President of the Scientific and Organizing Committee of 1EESRC

10:00-10:15 Coffee break

SESSION I Plenary MAIN HALL

Chair: A. Montone, N. Ignjatović

10:15-11:00 **MECANOCHEMISTRY UNDER HYDROGEN GAS: POTENTIALITIES FOR THE SINTHESYS OF EFFICIENT HYDROGEN STORAGE MATERIALS**
Fermin Cuevas, Junxian Zhang, Michel Latroche
Institut de Chimie et des Matériaux Paris-Est, CNRS-UPEC, UMR7182, 2-8 rue Henri Dunant, 94320, Thiais Cedex, France

11:00-11:45 **KEY CONCEPTS IN THE DESIGN OF FUNCTIONAL NANOPARTICLES**
Vuk Uskoković
Therapeutic Micro and Nanotechnology Laboratory, Department of Bioengineering and Therapeutic Sciences, University of California San Francisco, 1700 4th Street, San Francisco, CA 94158-2330, USA

11:45-12:30 **WHAT WE LEARN FROM THE HISTORY TO MASTER THE FUTURE: THE ROLE OF HYDROGEN**
Andreas Züttel
EMPA, Materials Science & Technology, Dübendorf, Switzerland

12:30-14:00 Lunch break

SESSION II Complex Hydride and MOFS HALL 8

Chair: E. Callini, S. Milošević, M. Lelis

14:00-14:25 **POLYMORPHISM AND STABILITY OF MAGNESIUM BOROHYDRIDE**

V. Ban[1], R. Černý[2], B. Richter[3], T.R. Jensen[3], C.J. Webb[4], Y. Filinchuk[1]

[1]Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Place L. Pasteur 1, 1348 Louvain-la-Neuve, Belgium; [2]Laboratory of Crystallography, Université de Genève, 24 quai Ernest Ansermet, 1211 Genève, Switzerland; [3]Center for Materials Crystallography, Interdisciplinary Nanoscience Center & Dept. of Chemistry, Aarhus University, Langelandsgade 140, 8000 Aarhus C, Denmark, [4]Queensland Micro- and Nanotechnology Centre, Griffith University, Nathan 4111, Brisbane, Australia

14:25-14:50 **ACHIEVING HIGH CAPACITY REVERSIBLE HYDROGEN STORAGE: $NaBH_4$@Ni CORE-SHELL NANOPARTICLES**

Meganne Christian, Kondo-François Aguey-Zinsou

Merlin Group, ARC Centre for Functional Nanomaterials, School of Chemical Engineering, The University of New South Wales, Sydney NSW 2052, Australia

14:50-15:15 **HYDRAZINE BORANE AND DERIVATIVES AS CHEMICAL HYDROGEN STORAGE MATERIALS**

Romain Moury, Umit B. Demirci, Philippe Miele

IEM (Institut Europeen des Membranes), UMR 5635 (CNRS-ENSCM-UM2), Universite Montpellier 2, Place E. Bataillon, F- 34095, Montpellier, France

15:15-15:30 **PHYSICAL AND CHEMICAL PROPERTIES OF VOLATILE COMPLEX HYDRIDES**

E. Callini[1], A. Borgschulte[1], I. Lindemann[2], A.J. Ramirez-Cuesta[3], M. Chong[4], C.M. Jensen[4], O. Gutfleisch[2,5], A. Züttel[1]

[1]Empa, Materials Sciences and Technology, CH-8600 Dübendorf, Switzerland; [2]IFW Dresden, Helmholtzstrasse 20, D-01069 Dresden, Germany; [3]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, United Kingdom; [4]Univ Hawaii Manoa, Dept Chem, Honolulu, HI 96822 USA, [5]Technische Universität Darmstadt, Petersenstrasse 23, 64287 Darmstadt, Germany

15:30-15:45 **TUNING THE HYDROGEN STORAGE OF MOFS BY INTRODUCING METALS ON THE LINKER SIDE**

Petra Ágota Szilágyi, Jana-Juan Alcañiz, Jorge Gascon, Hans Geerlings, Bernard Dam
Delft University of Technology, Netherlands

15:45-16:00 Coffee break

SESSION III Various Problems in Hydrogen Application HALL 8

Chair: Ž. Rašković-Lovre, A. Bliersbach, D. Mirabile Gattia

16:00-16:25 **THE EFFECTS OF SI AND EXPANDED PTFE SUBSTRATES ON FORMATION AND HYDROGENATION OF Mg AND Mg-Ti FILMS**

M. Lelis[1,2], D. Milcius[1], R. Zostautiene[3]
[1]Lithuanian Energy Institute, Breslaujos st.3, LT-44403 Kaunas, Lithuania;
[2]Vytautas Magnus University, Vileikos st. 8, LT-44404 Kaunas, Lithuania;
[3]Kaunas University of Technology, K.Donelaičio st.73, LT-44029 Kaunas, Lithuania

16:25-16:50 **METAL HYDRIDE FILMS FOR OPTO-ELECTRONIC APPLICATIONS**

Trygve Mongstad
Institute for Energy Technology, Norway

16:50-17:15 **LASER SURFACE MODIFICATION OF MATERIALS**

Sumsun Naher
Faculty of Engineering and Computing, Dublin City University, Dublin 9, Ireland

17:15-17:40 **MODIFICATIONS IN MICROSTRUCTURE OF MgH_2-BASED COMPOSITE UPON HYDROGEN CYCLING**

A. Montone, A. Aurora, **D. Mirabile Gattia**, M. Vittori Antisari
ENEA – R.C. Casaccia –Technical Unit of Materials - Via Anguillarese, 301 00123 Rome, Italy

20-22h Conference dinner HOTEL MOSKVA

Tuesday, 4th December 2012.

8:30-9:00 **Registration**

SESSION IV Hydrogen in Alloys HALL 8

Chair: M. Ponthieu, M. Sahlberg, S. Kurko

9:00-9:25 **SYNTHESIS AND HYDROGENATION OF $Mg_6Pd_{1-x}TM_x$ (TM =Ag, Cu) NOVEL SYSTEMS**

M. Ponthieu[1,2], J. F. Fernandez[1], F. Cuevas[2], J.R. Ares[1], P. Adeva[3], C. Sanchez[1]

[1]MIRE, Dpto. Física de Materiales, Facultad de Ciencias, Universidad Autónoma de Madrid, 28049, Madrid, Spain; [2]ICMPE/CNRS-UPEC UMR 7182, 2-8 rue Henri Dunant, 94320 Thiais Cedex, France; [3]Department of Physical Metallurgy, CENIM-CSIC, Av. De Gregorio del Amo 8, 28040 Madrid, Spain

9:25-9:50 **STRUCTURE AND HYDROGEN STORAGE PROPERTIES OF THE HEXAGONAL LAVES PHASE $Sc(Al_{1-X}Ni_X)_2$**

Martin Sahlberg

Department of Chemistry – Ångström Laboratory, Uppsala University, Box 538, SE-751 21 Uppsala, Sweden

9:50-10:15 **MICROSTRUCTURE EVOLUTION IN THE CHIPS OF Mg-10 at.% Ni ALLOY DURING HYDROGENATION**

Larisa Popilevsky[1], Vladimir Skripnyuk[1], Yuri Estrin[2], A.K. Dahle[3], Eugen Rabkin[1]

[1]Department of Materials Science and Engineering, Technion-Israel, Institute of Technology, Haifa, Israel; [2]Centre for Advanced Hybrid Materials, Monash University, Clayton, Victoria 3800, Australia; [3]Materials Engineering, The University of Queensland, Frak White Bldg. #43, Brisbane, QLD 4072, Australia

10:15-10:40 **COMBINATORIAL SYNTHESIS AND HIGH THROUGHPUT EXAMINATION OF HYDROGEN STORAGE ALLOY LIBRARIES**

M. Polanski, I. Kunce, J. Bystrzycki

Department of Advanced Materials and Technology, Military University of Technology, 2 Kaliskiego Str., 00-908 Warsaw, Poland

10:40-10:55 **STRUCTURAL CHARACTERIZATION AND ELECTROCHEMICAL HYDROGEN STORAGE PROPERTIES OF Ti_2Ni AND $(Ti_{1-x}Zr_x)_2Ni$ (x=0, 0.05, 0.1) ALLOYS PREPARED BY MECHANICAL ALLOYING**

Xianda Li[1], Omar Elkedim[1], M. Nowak[2], M. Jurczyk[2]

[1]FEMTO-ST, Fc-Lab, Université de Technologie de Belfort-Montbéliard, Site de Sévenans, 90010 Belfort cedex, France; [2]Institute of Materials Science and Engineering, Poznan University of Technology, Sklodowska-Curie 5 Sq., 60-965 Poznan, Poland

10:55-11:10 Coffee break

SESSION V Theoretical Investigation of Materials for Hydrogen Storage HALL 8

Chair: P. B. Jensen, R. Vujasin, N. Novaković

11:10-11:35 **HYDROGEN STORAGE PROPERTIES OF SUMANENE**

Stevan Armaković[1], Sanja J. Armaković[2], Jovan P. Šetrajčić[1,*]

[1]University of Novi Sad, Faculty of Sciences, Department of Physics, Trg Dositeja Obradovića 4, 21000, Novi Sad, Vojvodina, Serbia; [2]University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000, Novi Sad, Vojvodina, Serbia; [*]Academy of Sciences and Arts of Republic of Srpska, Bana Lazarevića 1, 78000 Banja Luka, Republic of Srpska, B&H

11:35-12:00 **INVESTIGATION OF SURFACE AND NEAR-SURFACE EFFECTS ON HYDROGEN DESORPTION PROPERTIES OF MgH_2**

Sandra Kurko, Sanja Milošević, Igor Milanović, Radojka Vujasin, Ljiljana Matović, Jasmina Grbović Novaković, Nikola Novaković

Vinča Institute of Nuclear Sciences, University of Belgrade, POB 522, 11000 Belgrade, Serbia

12:00-12:25 **COMPUTATONAL STUDY OF H STORAGE IN Pd AND Pt NANOPARTICLES SUPPORTED ON MgO**

Sergey M. Kozlov[1], Hristiyan A. Aleksandrov[1,2], Konstantin M. Neyman[1,3]

[1]Departament de Quimica Fisica and Institut de Quimica Teorica i Computacional (IQTCUB), Universitat de Barcelona, C/Marti Franques 1, 08028 Barcelona, Spain; [2]Faculty of Chemistry, University of Sofia, 1126 Sofia, Bulgaria; [3]Institucio Catalana de Recerca i Estudis Avançats (ICREA), 08010 Barcelona, Spain

12:25-12:40 **COMPUTATIONAL SCREENING OF MIXED METAL HALIDE AMMINES**

Peter Bjerre Jensen[1], Steen Lysgaard[1], Ulrich Quaade[2], Tejs Vegge[1]

[1]DTU Energy Conversion, Technical University of Denmark, Fysikvej 307, DK-2800 Kgs. Lyngby [2]Amminex A/S, Gladsaxevej 363, DK-2860 Søborg

12:40-12:55 **STRUCTURAL AND HYDROGEN SORPTION PROPERTIES OF $SmNi_{5x}Ga$ SYSTEM – AN EXPERIMENTAL AND THEORETICAL STUDY**

Nikola Biliškov, Goran I. Miletić, Ivka Štefanić, Antun Drašner

Laboratory of Solid State and Complex Compounds Chemistry, Division of Materials Chemistry, Ruđer Bošković Institute, Bijenička c. 54, HR-10000 Zagreb, Croatia

13:00-13:15 **NEWS FROM JEOL - ELECTRON MICROSCOPES AND SPECTROMETERS –** Slavko Žižek, univ.dipl.inž.el., Scan d.o.o **HALL 16**

12:55-14:00 Lunch break

SESSION VI Synthesis and Characterisation HALL 8

Chair: M. Polanski, H. Fahlquist, Lj. Matović

14:00-14:25 **INDUCTION PLASMA SYNTHESIS OF Mg_2Ni NANOPARTICLES FOR HYDROGEN STORAGE**

Burak Aktekin[1], Gülhan Çakmak[2],Tayfur Öztürk[1]

[1]Middle East Technical University, Metallurgical and Materials Eng. Dept., Ankara, Turkey; [2]Bülent Ecevit University, Metallurgical Eng. Dept., Zonguldak, Turkey

14:25-14:40 **POLYANIONIC GALLIUM-HYDROGEN CLUSTER IONS AS POSSIBLE INTERMEDIATES IN DEHYDROGENATION REACTIONS**

Henrik Fahlquist

Stockholm University, 106 91 Stockholm, Sweden

14:40-15:05 **EFFECT OF A $CaF_{2-X}H_X$ SOLID SOLUTION FORMATION IN THE MIXED SYSTEM CaH_2+CaF_2+MgB_2**

C. Pistidda[1], F. Karimi[1], S. Garroni[2], C. Milanese[3], L. Rude[4], J. Skibsted[4], T. R. Jensen[4], P. Nolis[5], C. Horstmann[1], C. Gundlach[6], M. D. Baró[7], T. Klassen[1], M. Dornheim[1]

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15:05-15:30 **DESIGN, SIMULATION AND OPTIMISATION OF AN ANODE SUPPORTED SOFC**

Hirad Azmin, Zahir Dehouche

School of Engineering and Design, Brunel University, Middlesex, UK

15:30-18:30 **SG MEETING** **HALL 8**

Chair: B. Paskaš Mamula, I. Milanović, Á. Kis-Tóth

16:15 -18:00 **POSTER SESSION** and coffee break

SASA Gallery of Science and Technology, Đure Jakšića 2

Wednesday, 5th December 2012.

9:00-9:30 Registration

SESSION VII Carbon Based Materials for Hydrogen Storage HALL 8

Chair: A. Ampoumogli, P. Javadian, A. Nale

9:30-9:55 **HYDROGEN STORAGE IN POROUS MEDIA AT ROOM TEMPERATURE**

Liga Grinberga, Janis Kleperis
Institute of Solid State Physics, University of Latvia, 8 Kengaraga Street, Riga, LV-1063, Latvia

9:55-10:20 **ENHANCING THE HYDROGEN CARBON INTERACTION**

Andreas Bliersbach
Empa, Swiss Federal Laboratories for Materials Science and Technology, Hydrogen and Energy, Überlandstrasse 129, CH-8600 Dübendorf, Switzerland

10:20-10:45 **HYDROGEN STORAGE PROPERTIES OF DIFFERENT METAL-DOPED CARBON-BASED COMPOSITES**

A. Ampoumogli[1], D. Giasafaki[1], A. Bourlinos[2], G. Charalambopoulou[1], A. Stubos[1], D. Gournis[3], Th. Steriotis[1]
[1]National Center for Scientific Research "Demokritos", Athens, Greece; [2]Department of Physics, University of Ioannina, Greece; [3]Department of Material Science Engineering, University of Ioannina, Greece

10:45-11:00 Coffee break

SESSION VIII Carbon Based Materials for Hydrogen Storage HALL 8

Chair: A. Ampoumogli, P. Javadian, A. Nale

11:00-11:25 **PRODUCTION OF SINGLE – WALL CARBON NANOTUBES BY KRF EXCIMER LASER ABLATION**

Petru-Marian Bota, Iulian Boerasu, Dorel Dorobantu, Dionezie Bojin, Marius Enachescu
Centre of Surface Science and Nanotechnology – University Politehnica of Bucharest, Splaiul Independentei 313, Bucharest, Romania

11:25-11:50 **CONFINEMENT OF $LiBH_4$ IN NANOPOROUS CARBON MATERIALS: SIZE AND INTERFACE EFFECTS ON HYDROGEN MOBILITY AND RELEASE**

A. Nale, P.E. de Jongh
Inorganic Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University, TB Utrecht, The Netherlands

11:50-12:15 **SCANDIUM FUNCTIONALIZED CARBON AEROGELS FOR HYDROGEN STORAGE**

Payam Javadian[1], Marek Polanski[2], Thomas Plocinski[2], Dariusz Zasada[2], Jerzy Bystrzycki[2], Flemming Besenbacher[3], Torben R. Jensen[1]
[1]Center for Energy Materials, Interdisciplinary Nanoscience Center (iNANO), and Department of Chemistry, Aarhus University, DK-8000 Aarhus, Denmark; [2]Faculty of Advanced Technology and Chemistry, Military University of Technology, 2 Kaliskiego Str., 00-908 Warsaw, Poland; [3]Interdisciplinary Nanoscience Center (iNANO) and Department of Physics and Astronomy, Aarhus University, DK-8000 Aarhus C, Denmark

12:15-12:30 **DEVELOPMENT OF NOVEL 3D TEM SAMPLE STRUCTURING METHODOLOGIES AND ADVANCED FIB AND TEM TOMOGRAPHY APPLICATIONS FOR NANOPOROUS MATERIALS**

Meltem Sezen
Sabanci University Nanotechnology Research and Application Center, Orhanli, Tuzla,34956 Istanbul, Turkey

12:30 Awards and closing ceremony

POSTER SESSION 1EESRC SASA Gallery of Science and Technology (Đure Jakšića 2)

NOTE: Please bring the posters to the conference registration desk on 03.12.2012

E1. HYDROGEN SORPTION PROPERTIES OF $MgH_2/NaBH_4$ COMPOSITES

Sandra Kurko[1], Annalisa Aurora[2], Daniele Mirabile Gattia[2], Vittoria Contini[2], Amelia Montone[2], Željka Rašković-Lovre[1], Jasmina Grbović Novaković[1]
[1]Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11000 Belgrade, Serbia, [2]ENEA, UTTMAT Research Centre of Casaccia, Via Anguillarese 301, 00123 Rome, Italy

E2. COMBINED SOLID STATE AND HIGH PRESSURE HYDROGEN STORAGE

Elisabeth Grube, Torben R. Jensen
Center for Energy Materials, Interdisciplinary Nanoscience Center, Department of Chemistry, Aarhus University, Langelandsgade 140, DK-8000 Aarhus, Denmark

E3. STRUCTURE AND HYDROGEN STORAGE PROPERTIES OF HIGH ENTROPY TIVCRNIFE AND TiVCrNiFeZr ALLOYS SYNTHESIZED BY USING LASER ENGINEERED NET SHAPING (LENS)

I. Kunce, M. Polanski, J. Bystrzycki
Department of Advanced Materials and Technology, Military University of Technology, 2 Kaliskiego Str., 00-908 Warsaw, Poland

E4. CHARACTERIZATION OF MULTILAYERED HYDROGEN STORAGE MATERIALS BY TRANSMISSION ELECTRON MICROSCOPY

Tyché Perkisas[1], Sara Bals[1], Lennard Mooij[2], Bernard Dam[2]
[1]Electron Microscopy for Materials Research (EMAT), University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium, [2]Department of Chemical Engineering, Delft University of Technology, Julianalaan 136, 2628 BL, Delft, The Netherlands

E5. ELECTRONIC STRUCTURE AND FORMATION ENERGIES OF HfV_2H_X LAVES PHASE

Jana Radaković, Jelena Belošević-Čavor, Vasil Koteski, Katarina Ćirić
Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11000 Belgrade, Serbia

E6. STRUCTURAL AND ELECTRONIC FACTORS GOVERNING HYDROGEN STORAGE PROPERTIES OF TMNi COMPOUNDS (TM=Ti, Zr, Hf)

Katarina Ćirić, Jana Radaković, Vasil Koteski, Dragica Stojić
Laboratory for Nuclear and Plasma Physics, Vinča Institute of Nuclear Sciences ,University of Belgrade, P.O. Box 522, 11000 Belgrade, Serbia

E7. HYDROGEN STORAGE, MICROSTRUCTURE AND MECHANICAL PROPERTIES OF $Mg_{65}Ni_{20}Cu_5Y_{10}$ METALLIC GLASS DEFORMED BY HIGH-PRESSURE TORSION

Á. Révész[1], **Á. Kis-Tóth**[1,*], L.K. Varga[2], E. Schafler[3], T. Spassov[4]
[1]Department of Materials Physics, Eötvös University, Budapest, H-1518, P.O.B. 32, Budapest, Hungary,[2]Research Institute for Solid state Physics and Optics, Hungarian Academy of Sciences.H-1525 Budapest, P.O.B. 49, Hungary,[3]Physics of Nanostructured Materials, Faculty of Physics, University of Vienna, A-1090 Vienna, Austria, [4]Department of Chemistry, University of Sofia "St. Kl. Ohridski", 1 J. Bourchier str., 1164 Sofia, Bulgaria

E8. EFFECTS OF PARTICLE SIZE AND TYPE OF CONDUCTIVE ADDITIVE ON THE ELECTRODE PERFORMANCES OF GAS ATOMIZED AB_5-TYPE HYDROGEN STORAGE ALLOY

L. Scherbakova, **M. Spodaryk**, Yu Solonin, A. Samelyuk
Institute for Problems of Materials Science (NASU), Krzhizhanovsky str., 3, Kyiv, Ukraine

E9. HYDROGEN DESORPTION PROPERTIES OF $MgH_2/LiAlH_4$ COMPOSITES

Igor Milanović[1], Sanja Milošević[1], Ljiljana Matović[1], Radojka Vujasin[1], Nikola Novaković[1], Riccardo Checchetto[2], Jasmina Grbović Novaković[1]
[1]Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11000 Belgrade, Serbia, [2]Faculty of Physics, University of Trento, 38123 Povo, Italy

E10. EVALUATION OF THE HYDROGEN EMBRITTLEMENT OF METALLIC MEMBRANES BY THE DISK TEST METHOD

A. Metallari, I. Markja
Polytechnic University of Tirana, Albania

E11. ELECTRONIC STRUCTURE AND CHARGE TOPOLOGY STUDY OF ALKALI HYDRIDES

Bojana Paskaš Mamula, Mirjana Medić, Bojana Kuzmanović, Ivana Radisavljević, Nenad Ivanović, Nikola Novaković
Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

E12. REACTIVELY DEPOSITED THIN FILMS OF MAGNESIUM NICKEL HYDRIDE

Željka Rašković-Lovre[1], Trygve Mongstad[2], Simon Lindberg[3], Stefano Deledda[2], Smagul Karazhanov[2]
[1]Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 552, Belgrade, Serbia, [2]Institute for Energy Technology, Box 40, NO-2027 Kjeller, Norway, [3]Chalmers University of Technology, SE-412 96 Gothenburg, Sweden

E13. INVESTIGATION OF NUCLEATION PROCESS IN MgH_2 THIN FILMS

Željka Rašković-Lovre[1], Sandra Kurko[1], Nenad Ivanović[1], Jasmina Grbović Novaković[1], Jose Francisco Fernández[2], Jose Ramon Ares Fernández[2], Carlos Sánchez[2], Nikola Novaković[1]

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E14. PREPARATION AND CHARACTERIZATION OF MgH_2-BASED COMPOSITE PELLETS

D. Mirabile Gattia[1], A. Montone[1], L. Pasquini[2]

[1]ENEA – R.C. Casaccia –Technical Unit of Materials - Via Anguillarese, 301 00123 Rome, Italy, [2]Department of Physics and CNISM, University of Bologna, V. Berti-Pichat 6/2, 40127 Bologna, Italy

E15. HYDROGEN-INDUCED DEFECTS IN THIN FILMS CHARACTERIZED BY VARIABLE ENERGY SLOW POSITRON ANNIHILATION SPECTROSCOPY

O. Melikhova[1], J. Cizek[1], W. Anwand[2], G. Brauer[2]

[1]Charles University in Prague, Faculty of Mathematics and Physics, V Holesovickach 2, CZ-180 00 Praha 8, Czech Republic, [2]Institut für Strahlenphysik, Helmholtz-Zentrum Dresden-Rossendorf, PO Box 510 119, D-01314 Dresden, Germany

E16. MAGNESIUM NANOPARTICLES AND NANODOTS: SYNTHESIS, STRUCTURE AND HYDROGEN SORPTION

Mattia Sacchi[1], Alan Molinari[1,2], Horst Hahn[2], Christiaan Boelsma[3], Bernard Dam[3], **Luca Pasquini**[1]

[1]Department of Physics and Astronomy, University of Bologna, v. Berti-Pichat 6/2, 40127 Bologna, Italy, [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany, [3]Department of Chemical Engineering, Faculty of Applied Sciences, Delft University of Technology, Julianalaan 136, 2628BL Delft, The Netherlands

E17. VANADIUM OXIDE AS HYDROGEN TECHNOLOGY MATERIAL

Dragica M. Minić[1], Dejan G. Minić[2], **Vladimir A. Blagojević**[1,3]

[1]University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, [2]Kontrola LLC, Austin, TX, USA, [3]Vida Holdings Corp. Ltd, Toronto, Ontario, Canada

E18. POSSIBLE PATHS OF HYDROGEN DIFFUSION IN TiO_2 – ROLE OF THE SURFACE

Radojka Vujasin, Igor Milanović, Sandra Kurko, Bojana Paskaš Mamula, Nikola Novaković

Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

E19. DESORPTION PROPERTIES OF MgH_2DESTABILIZED WITH $NaNH_2$ CATALYST

Sanja Milošević[1], Igor Milanović[1], Bojana Paskaš Mamula[1], Anđelka Đukić[1], Ljiljana Matović[1], Jasmina Grbović Novaković[1], Luca Pasquini[2]

[1]Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11000 Belgrade, Serbia, [2]Dipartimento di Fisica, Universita di Bologna and CNISM, v.le Berti-Pichat 6/2, I-40127 Bologna, Italy

E20.MICROSTRUCTURE OF ULTRAFINE-GRAINED WE43+12wt% Zn MAGNESIUM ALLOY AFTER EQUAL CHANNEL ANGULAR PRESSING

Jan Duchoň, Aleš Jäger, Viera Gärtnerová

Institute of Physics ASCR, v. v. i., Na Slovance 1999/2, 182 21 Praha 8, Czech Republic

E21. SEVERE PLASTIC DEFORMATION OF Mg-Mn ALLOY AT ROOM TEMPERATURE

Erik Švec, Jan Duchoň, Viera Gärtnerová, Aleš Jäger

Institute of Physics of the AS CR, v.v.i., Na Slovance 2, 182 21 Prague 8, Czech Republic

E22.ENHANCING THE HYDROGEN GRAPHENE INTERACTION BY METAL DECORATION

Andreas Bliersbach

Empa, Swiss Federal Laboratories for Materials Science and Technology, Hydrogen and Energy, Überlandstrasse 129, CH-8600 Dübendorf, Switzerland

E23.THE POTENTIAL APPLICATION OF HYDROGEN IN DEVELOPING COUNTRIES

Rabah Arkam

Euro T-Systems, 05, rue Chafai Ahmed, Tizi Ouzou Algeria

THE BOOK OF ABSTRACTS

P 1

MECANOCHEMISTRY UNDER HYDROGEN GAS: POTENTIALITIES FOR THE SINTHESYS OF EFFICIENT HYDROGEN STORAGE MATERIALS

Fermin Cuevas, Junxian Zhang, Michel Latroche

Institut de Chimie et des Matériaux Paris-Est, CNRS-UPEC, UMR7182, 2-8 rue Henri Dunant, 94320, Thiais Cedex, France

Mechanochemistry of hydrides by mechanical milling of metal powders under hydrogen gas is a powerful technique for the synthesis of metallic and complex hydrides (J. Huot *et al.* Prog. Mater. Sci.,58 (2013) 30). We review the historical advances on this technique and the current state-of-the-art. The synthesis of binary metal hydrides, solid solution BCC hydrides, hydrides from non-miscible metals, Mg- and alanate-complex hydrides is surveyed. Some particular phenomena such as ball-milling induced amorphisation, formation of metastable phases, multi-step reactions and incomplete hydride formation are reported. The obtained hydrides are typically nanocrystalline materials leading to fast kinetic reactions for hydrogen storage applications.

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P 2

KEY CONCEPTS IN THE DESIGN OF FUNCTIONAL NANOPARTICLES

Vuk Uskoković

Therapeutic Micro and Nanotechnology Laboratory, Department of Bioengineering and Therapeutic Sciences, University of California San Francisco, 1700 4th Street, San Francisco, CA 94158-2330, USA

Nanomaterials are defined as solid physical structures whose critical sizes do not exceed 100 nm. In this presentation, the origins of the field of nanoscience will be discussed, alongside some of the essential concepts applicable in the design of functional nanoparticles. Results obtained over years during the lecturer's research in various materials science fields - ranging from the synthesis of magnetic nanoparticles in reverse micelles, to nanostructured manganites for biomedical applications, to the chemistry of precipitation of cholesterol, to biomimicry of nanohierarchically organized hard tissues, to controlled delivery of proteins and small therapeutic molecules using silicon nanowires and calcium phosphate nanoparticles - will be mentioned and placed in a broader context defined by the role, the significance, the prospects and the tools of the field of nanoscience and nanotechnologies.

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P 3

WHAT WE LEARN FROM THE HISTORY TO MASTER THE FUTURE: THE ROLE OF HYDROGEN

Andreas Züttel

EMPA Materials Science & Technology, Dübendorf, Switzerland

The worldwide energy demand increases just as rapidly as the average temperature of the atmosphere. The reserves of fossil fuels worldwide are limited and the combustion of the carbon fuels leads to a severe increase of the CO_2 concentration in the atmosphere. The latter is responsible for the climate change. The future of the industrialized word, i.e. the economy as well as the society, is determined by the ability to change from fossil fuels as energy carriers to renewable energy. The main difference between the fossil period and the future is that renewable energy occurs as energy fluxes and, therefore, an energy carrier has to be synthesized.

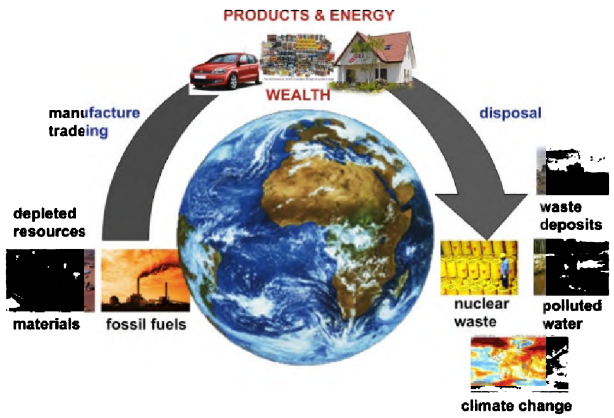

Fig. 1 Schematic representation of the economic system of the 20th century.

Hydrogen as an energy carrier can be produced and used in a purely technical and closed cycle. The storage of hydrogen in metals and complex hydrides as stable compounds offers a great volumetric storage density, however the gravimetric storage density is limited to less than 20mass% in the materials. In order to replace fossil fuels without scarification on energy density synthetic fuels based on hydrogen e.g. NH_3 or C_8H_{18} have to be developed. The latter also represents a effective CO_2 sink for the atmosphere if more is produced than used.

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TM 1

EFFECTS OF FULLERENOL NANO PARTICLES $C_{60}(OH)_{24}$ ON FILAMENTOUS FUNGUS *Aspergillus niger* Tiegh

Nikola Unković[1], Miloš Stupar[1], Milica Ljaljević Grbić[1], Jelena Vukojević[1], Marina Seke[2], Danica Jović[2], Aleksandar Djordjević[2]

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[2]Faculty of Science, Department of Chemistry, Biochemistry and Environment, Trg Dositeja Obradovića 3, 21000 Novi Sad, University of Novi Sad

The aim of this research is to investigate the effect of polyhydroxylated fullerene derivative, fullerenol $C_{60}(OH)_{24}$ nano particles (FNP), on mycelial growth and spore germination of model organism, filamentous fungus, *Aspergillus niger*. The effect of FNP was tested using microdilution method and spore germination assay. Here, we reported inhibitory effect of FNP on spore germination relative to the FNP concentration, as well as influence on morphophysiological characteristics of conidiogenus apparatus of *A. niger*. The most significant result is the depigmentation of the melanized conidial apparatus, since the melanin is the virulence factor in human pathogenic fungi.

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TM 2

PHASE AND MICROSTRUCTURAL EVOLUTION DURING SINTERING OF Zr-DOPED HYDROXYAPATITE

Miodrag J. Lukić[1], Smilja Marković[1], Srečo Davor Škapin[2], Dragan Uskoković[1]

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[2]Institute Jozef Stefan, Ljubljana, Slovenia

Doping of hydroxyapatite crystal structure with various ions is generally performed to improve biological, electrical, optical and mechanical properties of initial system. In this study, hydroxyapatite nanopowders doped with different amounts of zirconium (0, 1, 5, 10 at. %) have been sintered at different temperatures. Phase and microstructural evolution were examined by X-ray diffraction studies and field emission scanning electron microscopy.

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TM 3

THE BIOACTIVITY INVESTIGATION OF ELECTRODEPOSITED SILVER/HYDROXYAPATITE/LIGNIN COATINGS IN SIMULATED BODY FLUID

Sanja Eraković[1], Ana Janković[1], Ivana Matić[2], Zorica Juranić[2], Maja Vukašinović-Sekulić[1], Tatjana Stevanović[3], Vesna Mišković-Stanković[1]

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[2]Institute of Oncology and Radiology of Serbia, University of Belgrade, Belgrade, Serbia;
[3]Département des sciences du bois et de la forêt, Université Laval, Québec, Canada

The newest research on hydroxyapatite/lignin (HAP/Lig) scaffolds that assist bone repair refer us to employ organosolv lignin as the most suitable component for HAP composite that would provide better interconnected porous structure. The development of HAP composites containing Ag is necessary to improve antimicrobial activity of HAP composites. The Ag/HAP/Lig coatings were obtained by cathaphoretic deposition on Ti and characterized by various techniques in order to investigate the surface composition, structure and electrochemical characteristics as a function of soaking time in simulated body fluid (SBF). The coatings showed antibacterial properties, low toxicity, high bioactivity and corrosion stability in SBF.

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TM 4

PRODUCTION AND ANTIMICROBIAL ACTIVITY OF FIBERS BASED ON ALGINATE WITH INCORPORATED SILVER NANOPARTICLES

Srđan Vidović, Milan Stevanović, Maja Vukašinović-Sekulić, Bojana Obradović

Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia

The aim of our study was to investigate possibilities for production of hydrogels in the form of fibers based on alginate and poly(vinyl alcohol) (PVA) with incorporated silver nanoparticles (AgNPs) for potential use as antimicrobial wound dressings. Wet-spinning process was developed for production of nanocomposite Ag/alginate microfibers (~ 300 μm in diameter) as well as Ag/alginate/PVA fibers (~ 1mm in diameter) with incorporated electrochemically synthesized AgNPs at the concentrations of 1 and 2.6 mM, respectively. Antimicrobial activity of the obtained fibers in wet and dried forms, was investigated against E. coli and St. aureus revealing bacteriostatic and bactericidal effects

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TM 5

EVALUATION OF NOVEL Ag/ALGINATE MICROBEADS FOR POTENTIAL BIOMEDICAL APPLICATIONS

Jasmina Stojkovska, Željka Jovanović, Danijela Kostić, Maja Vukašinović-Sekulić, Vesna Mišković-Stanković, Bojana Obradović

Faculty of Technology and Metallurgy, University of Belgrade
Karnegijeva 4, 11120 Belgrade, Serbia

In this study, we have produced and characterized alginate microbeads with incorporated silver nanoparticles aimed for biomedical applications, specifically as potential antimicrobial wound dressings and soft tissue implants. Therefore, Ag/alginate microbeads were studied regarding the release of silver nanoparticles and/or ions, antibacterial activity against *Staphilococcus aureus* and cytotoxicity in monolayers of bovine calf chondrocytes. Furthermore, a short-term cultivation study of microbeads with immobilized chondrocytes mixed with nanocomposite microbeads under biomimetic bioreactor conditions was performed mimicking potential applications as engineered tissue implants. Overall results have shown potentials of Ag/alginate microbeads for biomedical applications, possibly reducing the need for antibiotics.

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TM 6

COPPER – ALGINATE MICROBEADS: BIOACTIVE, ANTIMICROBIAL BIOMATERIALS FOR POTENTIAL BIOMEDICAL APPLICATIONS

Ivana Madžovska, Maja Vukašinović – Sekulić, Bojana Obradović

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Bioactivity and antimicrobial properties of alginate hydrogels can be enhanced by using Cu^{2+} ions as cross-linking agents. In this study, Cu-alginate microbeads were produced by electrostatic extrusion of Na-alginate solution using $CuSO_4$ as a gelling agent at different concentrations. The increase in $CuSO_4$ concentration was shown to increase the cation content and mechanical properties, while decreasing the size of the obtained microbeads. Cu-alginate microbeads also exhibited antibacterial activity against *Staphylococcus aureus* and *Escherichia coli*. The obtained results imply that the presented production procedure could be optimized so to control the Cu^{2+} ion release aiming to induce desired biological responses.

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TM 7

HEMOLYTIC ACTIVITY OF BIOACTIVE NANOCOMPOSITES

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Huge range of tested biomaterials in recent decades has emerged as an ideal scaffold for cell growth, but few have demonstrated clinical efficacy. Among them, synthetic hydroxyapatite (HAp, $Ca_{10}(PO_4)_6(OH)_2$) is the most promising because of its biocompatibility, bioactivity, and osteoconductivity. Biocompatibility represents the primary concern for any material to be used as a substitute for natural tissue. Hydroxyapatite particles interact with numerous cellular systems in vivo, and some of these interactions may lead to cell damage and to stimulate platelet activation, coagulation and thrombus formation. The aim of this work was to examine the hemocompatibility of nano-calcium hydroxyapatite substituted with 5% and 12% cobalt (Ca /Co-HAp) and hydroxyapatite/poly-lactid-coglicolid (HAp / PLGA) in relation to pure HAp by testing their hemolytic activities. The results show the discrepancy in hemolytic activity of implanted matherials. The degree of crystallinity of samples had a more dominant influence on hemolysis than the percentage of substituted cobalt. Hemolysis ratios of the nano-calcium hydroxyapatite substituted with cobalt samples were below 3%, indicating good blood compatibility and that they are promising for medical application.

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TM 8

CHRONOAMPEROMETRIC DETERMINATION OF HYDROGEN-PEROXIDE BY MULTIWALL CARBON NANOTUBES MODIFIED CARBON BASED ELECTRODES

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Nowadays, multiwall carbon nanotubes (MWCNT) are very popular material for designing of amperometric sensors and biosensors. The aim of this work was to investigate the applicability of multiwall carbon nanotubes modified carbon paste electrodes (MWCNT-CPE) and screen printed carbon electrodes (MWCNT-SPCE) for the chronoamperometric monitoring of hydrogen-peroxide concentration in model systems. As first, optimization experiments were performed to prepare carbon paste electrodes (based on graphite powder and paraffin oil) bulk doped with unmodified (MWCNT-CPE) and chemically oxidized multi-walled carbon nanotubes (C-MWCNT-CPE). The influence of the dopant nature (unmodified and oxidized forms) and content (5% and 10% w/w) were investigated. Based on the results, 5% w/w of unmodified MWCNT in MWCNT-CPE showed better analytical performances in terms of hydrogen-peroxide determination than the unmodified CPE, and the C-MWCNT-CPE, because of lower noise and higher sensitivity and reproducibility of the developed analytical method. In our preliminary work, MWCNT-SPCE was also tested for chronoamperometric determination of hydrogen-peroxide.

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TM 9

ELECTROCHEMICAL SYNTHESIS AND CHARACTERIZATION OF SILVER NANOPARTICLES IN POLY(VINYL ALCOHOL) SOLUTION

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In this work, the optimal conditions for the electrochemical synthesis of silver nanoparticles in the solution of poly(vinyl alcohol), PVA, were investigated, by varying the values of the applied current density, ranging from 5 to 50 mA cm^{-2}. The galvanostatic synthesis is performed using aqueous solutions of 10 wt. % PVA, containing KNO_3 and $AgNO_3$. The presence of silver nanoparticles was confirmed by UV-vis spectroscopy. TEM analysis shows that the obtained silver nanoparticles were spherically shaped. FTIR spectroscopy indicates the interactions between silver nanoparticles and PVA molecules.

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TM 10

VOLTAMMETRIC DETERMINATION OF DOXORUBICIN BY RENEWABLE SILVER-AMALGAM FILM ELECTRODE

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Voltammetric characterization and determination of Doxorubicin (DOX) was performed by direct cathodic square-wave voltammetry (SWV) and by a highly-sensitive adsorptive stripping square-wave voltammetry (SWAdSV) using renewable silver-amalgam film electrode (Hg(Ag)FE) in aqueous Britton-Robinson buffer solution as supporting electrolyte. In the investigated pH range between 2.0 and 8.0, the reduction peak of DOX was obtained in the interval of approximately -0.3 to -0.8 V. At pH 6.0 Hg(Ag)FE showed best analytical characteristics in respect of the reduction peak shape and intensity of DOX. The developed SWAdSV method was used to determine of target analyte in model solutions in the concentration range of 4,99-59,64 ng ml^{-1}.

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TM 11

CORROSION AND ION RELEASE BEHAVIOR OF NITRIC ACID PASSIVATED STAINLESS STEEL

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The aim of this work was to identify the effects of stainless steel surface passivation on corrosion and release ion behavior. Cylindrical samples were wet ground, polished, rinsed with water and washed with ethanol in the ultrasonic cleaner. The samples were divided into 3 treatment groups: non-treated, treated with the nitric acid (65 %) 15 min and treated with the acid 30 minutes. Corrosion resistance of samples was determined by performing the potentiodynamic tests in Hank's solution at 37°C. Amount of released Ni, Cr and Fe ions in mg/dm^3 was appointed right after treatment and cleaning. Obtained results indicate the passivation of the stainless steel could improve itscorrosion resistance and decrease amount of metal ion released from the surfaces.

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TM 12

VOLTAMMETRIC DETERMINATION OF FENOXANIL FUNGICIDE BY RENEWABLE SILVER-AMALGAM FILM ELECTRODE

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Environmental friendly direct cathodic square-wave voltammetric (SWV) and adsorptive stripping square-wave voltammetric (SWAdSV) methods using a renewable silver-amalgam film electrode (Hg(Ag)FE) were developed for the characterization and determination of Fenoxanil (Fen, *N*-(1-cyano-1,2-dimethylpropyl)-2-(2,4-dichlorophenoxy)propanamide) fungicide in aqueous Britton-Robinson buffer solution as supporting electrolyte. In the investigated pH range between 2.0 and 9.0, two reduction peaks were observed for Fen, one was at -0.4 V and another one at -1.5 V. For determination of Fen the second peak was selected. The well shaped and most intensive reduction signal was obtained at pH 6.0, so this pH was chosen for analytical purposes. Under the optimal conditions, there was a linear relationship between the reduction peak height and concentration of Fen over the concentration range of 2.72-15.46 μg mL^{-1} using SWV method and 0.71-2.29 μg mL^{-1} using SWAdSV one. Finally, the developed SWV and SWAdSV methods were tested to determine Fen in selected real samples.

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TM 13

CHARACTERIZATION OF ORGANIC INHIBITOR FOR CORROSION OF MILD STEEL IN 3 wt. % NaCl SOLUTION SATURATED WITH CO_2

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In this study talloil diethylenetriamine imidazoline (TOFA/DETA imidazoline) was evaluated as corrosion inhibitor for mild steel in 3 wt. % aqueous NaCl solution at 20°C and 70°C using the following techniques: the electrochemical impedance spectroscopy, linear polarization resistance and weight loss measurements. The adsorption process was followed by quartz crystal microbalance and the morphology of the steel surface was investigated by scanning electron microscopy and atomic force microscopy. All measurements applied indicated that TOFA/DETA imidazoline significantly decreased the corrosion rate when 70 ppm (vol.) of corrosion inhibitor was added due to its ability to adsorb on the metal surface.

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TM 14

THE INFLUENCE OF ADDITIVES ON THE MORPHOLOGICAL AND CORROSION PROPERTIES OF ELECTRODEPOSITED Zn-Mn ALLOYS

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The electrodeposition of Zn–Mn alloys in chloride electrolytes, as sacrificial coatings on steel, was investigated. It was found that depending on the plating parameters up to 36 at.% Mn could be obtained in Zn-Mn alloy coatings, however, at the cost of very low current efficiencies and with incorporation of a great amount of oxides/hydroxides. In order to prevent formation of oxides the addition of inhibitor for hydrogen evolution and surfactant was examined. Their effects upon the composition, morphology, microstructure and corrosion stability of the deposit were investigated using electrochemical methods, scanning electron microscopy and energy dispersive X-ray spectrometry.

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TM 15

IDENTIFICATION OF PROMISING CHEMICAL SYSTEMS FOR THE SYNTHESIS OF NEW MATERIALS STRUCTURE TYPES: AN *AB INITIO* MINIMIZATION DATA MINING APPROACH

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In this research we performed data exploring for binary compounds with elements from groups V, IV - VI, and III – VII, with the goal to identify chemical systems where the recently proposed "5-5" structure type might be experimentally accessible. Among others, TlF, SnO, SnS, SnSe, GeS, GeSe, PbO, PbS, ZnO and ZnS, were chosen for the study. In the next step, for each of these systems a local optimization on *ab initio* level with the LDA functional was performed for the 5-5 structure type plus other experimentally observed and theoretically proposed structure types, for comparison. Afterwards, the results were combined with earlier theoretical work involving the 5-5 structure in the earth alkaline metal oxides and the alkali metal halides. As a result, we suggest the GeSe and the ZnO systems as the most suitable ones for synthesizing the 5-5 structure type.

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TM 16

KINETICS OF CRYSTALLIZATION OF $Fe_{89.8}Ni_{1.5}Si_{5.2}B_3C_{0.5}$ AMORPHOUS ALLOY

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Kinetics of structural transformation of $Fe_{89.8}Ni_{1.5}Si_{5.2}B_3C_{0.5}$ amorphous alloy was examined using DSC measurements at different heating rates. Distinct peaks of glass transition and crystallization were observed. In order to understand crystallization process better, complex crystallization peak was deconvoluted into two steps, which correspond to the formation of α-Fe(Si) and Fe_2B crystalline phases. Kinetic triplets for both crystallization steps were determined, showing relatively high values of activation energies as a consequence of simultaneous movement of large number of atoms. Determination of the correct form of the conversion function revealed that Šesták-Berggren model best describes both crystallization steps.

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TM 17

CHARACTERIZATION OF PULSED LASER DEPOSITED CdS ON TiO_2 NANOTUBES ARRAYS

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Using field emission scanning electron microscopy and high resolution transmission electron microscopy with electron energy loss spectroscopy and energy filtered mode of transmission electron microscopy, the characterization of acquired samples was performed and the chemical mapping of the elements was obtained. The results showed that the samples consisted of highly oriented titania nanotube arrays with cadmium sulfide deposited inside and between nanotubes, which had a ~100 nm inner diameter. The deposition was performed via pulse laser deposition technique. The deposit thicknesses were ~ 5 nm and ~ 10 nm, increasing with the number of laser pulses, 250 and 500, respectively.

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TM 18

INFLUENCE OF PARTICLE SIZE AND MORPHOLOGY OF ZnO POWDERS ON THEIR OPTICAL PROPERTIES

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In this work we present details of different synthesis procedures for preparation of ZnO powders and a possibility to create various particles morphology and average size; from micrometer rods to nanometer spherical particles. We studied two synthesis methods, low temperature hydrothermal processing (HT) and ultrasound processing (US). The morphology and average particle size of the ZnO particles were modified by adjusting the mole ratio of $[Zn^{2+}]/[OH^-]$ in the reactants solution. Agglomeration of the particles was prevented using a polyvinyl pyrrolidone (PVP) as a capping agent. The synthesized powders were characterized by X-ray powder diffraction (XRD), scanning electron microscopy (FE SEM) and UV-Vis diffusion reflection spectroscopy (UV-Vis DRS). Based on the results of the scanning electron microscopy we proposed a possible growth mechanism of the ZnO particles depending on the mole ratio of $[Zn^{2+}]/[OH^-]$. Also, we considered the influence of particle size and morphology on the optical properties of the prepared powders. The observed results sowed that the size and morphology of ZnO particles greatly affect the absorption of visible light (%) and the shift of the energy gap (eV).

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TM 19

COMPACTION PRESSURE'S INFLUENCE ON DENSITY AND ELECTRICAL PROPERTIES OF SINTERED CORDIERITE-BASED CERAMICS

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Mechanical activation is widely used for sample preparation before the sintering process. However, the influence of pressure, which is used for compaction, has not been completely investigated. Cordierite, $2MgO{\cdot}2Al_2O_3{\cdot}5SiO_2$, is a very attractive high-temperature ceramic material, due to its outstanding electrical characteristics, such as the low temperature expansion coefficient, low dielectric constant and good mechanical properties. Based on our previous investigation, the mechanical activation of the starting mixtures with 5.00 mass% TiO_2 was performed in a high energy ball mill during 10 minutes. Compaction pressure varied from 0.5 to 6 t/cm^2. Differential thermal analysis (DTA) was used in order to determine characteristic temperatures within the system during heating. Sintering process was performed at 1350 ^oC for 4 h in air atmosphere. The phase composition of activated and sintered samples was analyzed by the X-ray diffraction method. Scanning electron microscopy was performed to analyze both compacted and sintered sample microstructure. This paper deals with the influence of compaction pressure on the densities of green bodies as well as on the sintered samples, along with electrical properties

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TM 20

DEPOSITION OF THE DLC STRUCTURES IN THE LOW-PRESSURE OXY-ACETYLENE FLAT FLAME

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The morphology and phase composition of the diamond-like carbon (DLC) structures as a function of the deposition process parameters are investigated. The DLC was deposited in the low-pressure oxy-acetylene flat flame onto molybdenum substrates. It was done with the designed flame burner by spreading the flame over the area of 40 mm in diameter with the overall acetylene and oxygen flow up to 4 l/min and by changing the substrate distance and the O_2/C_2H_2 ratio. The morphology and the phase composition of the DLC coatings significantly depend on the deposition process parameters, especially on the O_2/C_2H_2 ratio.

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TM 21

CHEMICAL STABILITY OF $Fex(Sb_2S_3)_{0.75}(SbI_3)_{0.25})_{1-x}$ GLASSES

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This paper presents the investigation of chemical stability of $Fe_x(Sb_2S_3)_{0.75}(SbI_3)_{0.25})_{1-x}$ chalcogenide glasses. The content of Fe vary from 0.01 to 5 at. %. The dissolution rates of investigated samples in potassium hydroxide solution of different concentrations at room temperature were calculated by measuring the mass loss. The samples showed relatively low dissolution rate, eg. large chemical stability but still lower than for the other chalcogenide glass systems. The dissolution rates increased with the increase of Fe concentration in the glass matrix, so the Fe atoms could be considered as catalysts for chemical dissolution.

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TM 22

WELDING PARAMETERS PREDICTION BY THE ANALYTICAL METHODS AND USE OF NUMERICAL SIMULATION SOFTWARE FOR GS-36Mn5 STEEL

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The use of cast steel GS 36Mn5 in the production of welded construction requires the use of special measures during welding process or surfacing, such as preheating, heat treatment after welding, the use of buffer layers and etc. Analytical assessment of the material weldability was performed with different methods and result comparation with the results of software application "Weld simulator" for MMA process. The results show good agreement in the assessment of welding parameters by applied procedures, and suggest what measures must be taken to obtainhigh quality of welded joints.

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TM 23

CALCULATION OF TEMPERATURE DISTRIBUTION OF THE POWDER PARTICLES IN THE SPRAY DEPOSITION PROCES

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A numerical simulation of spray deposition process for aluminum alloy onto rotating substrate is developed. For the modeling of ones was applied heat-flow analysis. The mathematical model was solved numerically. Temperature distribution for different particle size depending on the distance between the nozzle and the substrate is shown. Obtained results indicate the presence of smaller temperature gradients for the larger diameter particles.

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TM 24

APPLICATION OF FINITE ELEMENTS METHOD IN ANALYSIS OF DYNAMIC BEHAVIOR OF COMPOSITE LAMINATES

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This paper presents the theoretical bases of propagation of elastic waves in a composite laminate. According to theoretical assumptions the paper analyses the stress and displacement fields of a laminate which is modeled by orthotropic multilayer shell elements by using PAK software package. Finally the paper shows the comparative result of different orientations monolayers of laminates and different types of dynamic loading by using the implicit Newmark method and the explicit central difference method for numerical integration of dynamic equations of motion.

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TM 25

PROPAGATION OF BULK WAVES IN A TRANSVERSAL ISOTROPIC MEDIUM

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The present paper treats the fiber reinforced medium as a homogeneous transversally isotropic medium. In order to follow influence of fiber direction on mechanical properties, constitutive relations are modeled as a function of fiber direction in each point of continuous media.
Testing the mechanical behavior of an anisotropic medium with propagation of bulk waves is done using Riemann-Christoffel's equation that defines three homogeneous linear equations which determine displacements amplitudes. Thus the propagation of bulk waves is analyzed as a system of homogeneous linear equations and represents a condition of propagation. Characteristics of these waves are determined by relations between waves' propagation and constitutive characteristics of the medium. The results are numerically presented using the concept of slowness curves which are inverse velocity curves. The results are processed in Matlab software.

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TM 26

ON THE TRANSITION FROM DELOCALIZED TO LOCALIZED VIBRON STATES IN MACROMOLECULAR CHAINS

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In this paper, the nature of vibron excitation states in quasi-1D macromolecular chains is investigated. Our study makes use of the simple mean field approach, based on the usage of variational extension of the Lang-Firsov unitary transformation. We take into account vibron interaction with acoustical phonon modes. We find that quasi-free (Bloch-like) vibron states may occur at low temperature limit, but, increasing the system temperature, localized vibron states may appear.

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TM 27

SUBSTITUTION EFFECTS OF SUMANENE BENZYLIC POSITIONS WITH BORON AND NITROGEN ATOMS

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Sumanene is typical representative of molecular bowls, also known as buckybowls or π-bowls, which has three sp3 hybridized carbon atoms at the benzylic positions as characteristic structural feature. This specific structural property may allow functionalization of new bowl shaped structure.
In this work we investigated effects of substitution of carbon atoms of sumanene with boron and nitrogen atoms within DFT computations. We used quantum molecular descriptors in order to better understand sumanene molecule and the effects of substitution. Isomers obtained by substitution were further subjected to the study of NMR parameters, NICS, bowl-to-bowl inversion barrier, NBO/NPA analysis and DOS analysis.

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TM 28

THERMAL PROPERTIES OF CARBON NANOTUBES

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We study thermal expansions and thermal conductance of single-wall CNTs (carbon nanotubes) and helically coiled CNTs by using atomistic simulations techniques based on the Brenner interatomic potential. Model of helically coiled CNTs consists of periodically incorporated heptagons and pentagons into the hexagonal network. Initial atomic coordinates, which are further subjected to the optimization procedure, are generated with a help of the graph theory and topological coordinate method. Temperature dependence of geometrical parameters of the both systems is determined by minimizing Helmholtz free energy at a finite temperature. Local harmonic approximation with implementation of line group symmetry is used for calculation of Helmoltz free energy. Molecular dynamic simulations are applied to calculate thermal transport of CNTs. Coefficients of thermal conductance is obtained by Fourier's low. Direct method for calculation of thermal conduction is applied to simulate thermal energy transport of CNTs, which mimics the natural thermal transport process.

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TM 29

RAMAN SCATTERING STUDY OF IRON-CHALCOGENIDE SUPERCONDUCTORS

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Since the first report on superconductivity in LaOFeAs—known as the "1111" structure from its formula unit—at the end of February 2008, the iron pnictide superconductor family has been quickly expanded to different types of structures. Two certainly most intriguing are 11 and 122* iron chalcogenides.Here we present detailed analysis of the temperature dependent polarized Raman scattering spectra of $FeTe_{1-x}Se_x$ and $K_xFe_{2-y}Se_2$ based on the crystal structure peculiarities. In $K_xFe_{2-y}Se_2$ we found 16 Raman-active modes corresponding to the vibrations of the atoms of the I4/m symmetry structure. Two additional modes, for which we believe that originates from the vibrations within the FeSe layer of the I4/mmm symmetry, have also been observed. This shows the presence of phase separation between superconducting and isolating regions that occurs at nano-scale as a consequence of Fe vacancy ordering.

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TM 30

EFFECTS OF OPTICAL BEAM MULTIPLE REFLECTIONS TO PHOTOTHERMAL RESPONSE - CORRECTION FACTOR

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The theoretical model of optically induced surface temperature changes is presented, which includes multiple reflections of incident beam at the boundaries of a sample. The prediction of the model is compared with previous models and correction factor is derived. It is shown that this correction can affect the values of the surface temperature if the sample is optically transparent. The consequences of this correction are discussed to photothermal evaluation of optical coefficient of absorption and other properties of transparent and semi-transparent samples.

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TM 31

SIC MOSFET – MODEL OF CURRENT-VOLTAGE CHARACTERISTICS AND POSSIBILITIES FOR IT'S IMPLEMENTATION IN BIOMEDICAL ELECTRO EQUIPMENT

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In this paper, the new analytical model of SiC MOSFET current-voltage characteristics is proposed. Possibilities for SiC based MOSFET implementation in biomedical electro equipment are considered. To make a high current, high voltage power MOSFET (Metal Oxide Semiconductor Field Effect Transistor), silicon carbide (SiC) can be used. Unique semiconductor SiC possesses superior electronic properties such as high electron saturation drift velocity, high breakdown electric field, high thermal conductivity, wide band gap energy; SiC can be thermally oxidized etc. Thus, SiC MOSFET is employed as power electronic device. One of the most important MOSFET characteristics is its current – voltage characteristics (I – V characteristics). These characteristics depend on many parameters and parameters optimization requires great efforts. SiC MOSFETs can be used in biomedical electro devices which operate under extreme conditions.

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TM 32

STUDY OF THE SHUNGITE AND COANP STRUCTURES NONLINEAR PROPERTIES

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It is well known that carbon nanoobjects such as fullerenes, carbon nanotubes and graphene can activate the nonlinear properties of doped organic materials, which could be useful for power limiting application, for example, to protect the human eyes and photosensitive equipments. The aim of this study was an investigation the nonlinear properties of a natural material – shungite, which contains the fullerenes molecules, in comparison with 2-cyclooctylamino-5-nitropyridine (COANP) system. The suspensions of shungite in water and chloroform were used for measurements of output energy and calculations the attenuation of laser energy with wavelength 532 nm and pulse duration 10 ns. We have obtained the significant laser attenuation of shungite in water suspension. The same effect of decrease of laser power was observed in suspension with chloroform too. The results of our experiments can be explained by the changes of nonlinear parameters such as third-order nonlinear susceptibility and nonlinear refraction due to an existence of dipole moment in fullerene molecules and intrinsic the dipole moment of shungite. The explanation has been coincided with that made for COANP-fullerene system, which reveals the increased local volume polarizability testified via increased cubic nonlinearity.

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TM 33

STUDY OF THE CARBON NANOTUBES INFLUENCE ON THE REFLECTION SPECTRUM AND THE MICROHARDNESS OF KBr, BaF_2

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It is well known that the basic features of carbon nanotubes are regarded to their high conductivity, strong hardness of their C—C bonds as well as complicated and unique mechanisms of charge carrier moving. These peculiarities of carbon nanotubes and their possible optoelectronics application is placed under consideration of different scientific group are placed. In the current paper the effect of surface carbon nanotubes influence on the surface properties of the soft" materials of the UV and the IR spectral ranges are discussed. Among the materials the main aspect is given to the structures such as potassium bromide and barium fluoride. The spectral characteristics and mechanical features are considered. The correlation between spectral and mechanical parameters of the materials studied is shown. The possible areas of application are done.

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TM 34

TG-DTG STUDY OF BULK As_2S_3 CHALCOGENIDE GLASSES DOPED WITH BISMUTH

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Thermal properties of the glasses from the system $Bi_x(As_2S_3)_{100-x}$ with x = 0, 1.5, 3, 5 and 7 at. % Bi were studied by thermo gravimetric analysis. TG-DTG curves were measured using the device TA Instruments SDT Q600. Analysis of TG-DTG recordings for the samples at the same heating rate allowed characterization of the decomposition process and weight loss as a function of the content of doping atoms. A more complex decomposition process in the reference to other samples is observed for the sample with 7 at. % Bi, which can be explained by melting of the already existing crystallization centers in amorphous matrix. The presence of the crystallization centers in the glass $Bi_7(As_2S_3)_{93}$ is confirmed by the appearance of peaks on X-ray pattern of this sample. Identification of existing crystallization centers was carried out by X-ray analysis. The diffractograms of the other investigated samples from the system confirmed their amorphous character.

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TM 35

SYNTHESIS AND CHARACTERIZATION OF $NiFe_2O_4/BaTiO_3$ THIN FILMS

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Recently there has been great research interest in composite multiferroic materials with the coexistence of both magnetic and polarization ordering. Amoung them, multiferroic films with alternating ferrite and piezoelectric oxide layers have special importance since they are less leaky and facilitate on-chip integration. In this paper different multilayered $NiFe_2O_4/BaTiO_3$ (NFO/BTO) films were obtained on glass substrates by using dip and spin coating deposition techniques of different precursor solutions at room temperature. Two $NiFe_2O_4$ sols obtained from nickel and iron nitrate salts were examined, one dissolved in water at pH=3, while the second one was dissolved in 2-methoxyethanol with pH=1.8. $BaTiO_3$ acetate sol was obtained at room temperature by mixing of Ba^{2+} ions (from $BaCO_3$) dissolved in concentrated acetic acid with tetrabutyl-orthotitanate. Optimal processing conditions for the preparation of multilayered NFO/BTO films were investigated. Viscosity and particle size of precursor sols were monitored with time and thin films were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and atomic force microscopy (AFM). It was shown that the prepared films were crack-free, with the thickness of 100-400 nm, uniform surface texture and rounded grains having grain size in the nanometer range.

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TM 36

PHASE DIAGRAM OF SYSTEM $ZnGeAs_2$-$CdGeAs_2$

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The chalcopyrites $ZnGeAs_2$ and $CdGeAs_2$ are advanced materials for nonlinear optic applications. The interaction between $ZnGeAs_2$ and $CdGeAs_2$ was investigated with a view to create a new materials with widen range of energy gap and to choose the technological conditions of the $Zn_XCd_{1-X}GeAs_2$ solid solution single crystal growth. Eleven equilibrium samples of $Zn_XCd_{1-X}GeAs_2$ with interval 0.1 mol. were synthesised and studied by X-ray, DTA and microstructure analysises. Above 873 K solid solutions of $Zn_XCd_{1-X}GeAs_2$ take place in all range of the concentration. Lower of this temperature the decay's region was observed. The samples $ZnGeAs_2$ and $Zn_{0,9}Cd_{0,1}GeAs_2$ crystallized as chalcopyrite and sphalerite structures. The temperature of the phase transitions were 1123 K. The reported study was supported by RFBR, research project No 12-03-31203.

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TM 37

THE INFLUENCE OF THE STRUCTURE OF THE POLYBUTADIENE BLOCK TO THE MECHANICAL PROPERTIES OF THE POLYSTYRENE-b-POLYBUTADIENE-b-POLY(METHYL METHACRYLATE) COPOLYMER

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Triblock copolymers with the defined structure are the materials of the great importance in the class of elastic materials. Combining the hard, brittle block(s) with the block with the elastic properties, it is possible to get material with the wide range of properties and application. In this work, the influence of the structure of the elastic block to the macroscopic properties of the material was investigated. The mechanical properties were determined by the measurement of stress-strain diagram. In this series of experiments, it was found that higher amount of 1,4 butadiene causes moderate stress drops as well as the higher elongation.

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TM 38

INFLUENCE OF GOLD IONS IMPLANTATION AND OZONE TREATMENT ON SURFACE CHARACTERISTICS OF HIGH DENSITY POLYETHYLENE

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The aim of this work was to investigate possible effects of gold implantation and ultraviolet (UV) ozone treatment on surface characteristics of High Density Polyethylene (HDPE). HDPE had been modified by implantation of gold ions with the energies of 50 keV, 100 keV, 150 keV and 200 keV, and dose of $5 \cdot 10^{15}$ ions/cm^2. After implantation, the samples have been treated with UV ozone. Atomic force microscopy (AFM) topography images have shown significant changes of structure after implantation, and even more considerable changes after UV ozone treatment. UV ozone treatment caused significant changes of roughness on HDPE implanted with gold ions of the 150 keV and 200 keV energies. AFM phase imaging has shown that the surface composition is homogenous after implantation and UV ozone treatment. The analysis of the phase image histograms has shown that after implantation of gold ions the surface of HDPE becomes harder, with dominant elastic character, while UV ozone treatment causes softening of HDPE surface, i.e. dominant viscous character.

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TM 39

SURFACE DIELECTRIC PROPERTIES AND FOURIER TRANSFORM INFRARED (FTIR) SPECTROSCOPY SPECTRA OF LOW-DENSITY POLYETHYLENE (LDPE) ETCHED BY TRICHLOROACETIC ACID AT DIFFERENT TEMPERATURES

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Samples of LDPE were treated with Trichloroacetic acid for a period of one hour, at temperatures ranging from 20 to 70 °C. After the treatment, samples were analyzed with FTIR spectroscopy. FTIR measurements revealed chemical and crystallinity changes on the surface, as a direct result of the treatment. Surface dielectric properties of acid etched LDPE were analyzed in frequency range from 20 Hz to 200 kHz. In comparison to the untreated LDPE, the etched samples showed significantly different values of the conductance (G) at low frequencies. It was also observed, at higher frequencies, that an increase of the acid treatment temperature can result with lower values of conductance as well as susceptance (B) of LDPE with respect to the acid treatment at room temperature.

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TM 40

NOVEL ASYMMETRIC POLYETHERSULFONE MEMBRANES FOR ULTRAFILTRATION APPLICATION

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Ultrafiltration has recently become popular as a promising separation method in many industrial processes covering fractionation and concentration steps in the food, pharmaceutical and biotechnology industries as much as in water and wastewater treatments. This paper presents the synthesis of novel asymmetric polyethersulfone membranes containing an interpenetrating network of poly(glycidyl methacrylate) (PGMA). In order to improve the properties and application range of membranes, the epoxy groups from PGMA are converted to amine groups by ring opening under alkaline conditions. Membranes before and after functionalization are characterized by FTIR-ATR, elemental analysis and water permeability.

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TM 41

SURFACE MODIFICATION OF PECTIN SPHERES CROSS-LINKED IN LEAD (IV) AND COPPER(II) SOLUTIONS

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The purpose of this study was to investigate the surface modification of spherical pectin particles obtained during gelling pectin. Pectin was cross-linked in salt solutions of copper (II) and lead(IV). Depending on concentration (0.01, 0.05 and 0.1 moldm^{-3}) and type of salt dimensions and deviation from sphericity were measured. Sensitization and activation of the pectin spheres' surfaces was carried out in tin(II) chloride and palladium(II) chloride solutions (0.1 moldm^{-3}), respectively. In order to metallize them, the samples were treated in solution of silver(I) nitrate. For the characterization of the particles optical microscopy was used, and results were analyzed by image analysis.

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TM 42

FERROMAGNETIC POLYANILINE/TiO_2 NANOCOMPOSITES

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Novel ferromagnetic polyaniline PANI/ TiO_2 nanocomposites were synthesized by the oxidative polymerization of aniline with ammonium peroxydisulfate in an aqueous medium, in the presence of colloidal TiO_2 nanoparticles (d ~ 4.5 nm), without added acid. The morphological, magnetic, structural, and optical properties of the PANI/TiO_2 nanocomposites prepared at initial aniline/TiO_2 mole ratios 80, 40, and 20 were studied by scanning electron microscopy, superconducting quantum interference device, FTIR, Raman, and UV-Vis spectroscopies. The electrical conductivity of synthesized composites was ~10^{-3} Scm^{-1}. The room temperature ferromagnetic response was detected in all investigated PANI/TiO_2 nanocomposites.

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TM 43

COMPARISON OF DIELECTRIC PROPERTIES OF POLYVINYLIDENE FLUORIDE + Cu COMPOSITES MEASURED BY SINUSOIDAL AND TRIANGLE SIGNALS

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Comparative analysis of dielectric properties of Polyvinylidene fluoride (PVDF) + Cu composites has been done by applying sinusoidal and triangle electrical signals. Composite samples were processed from the PVDF solution with different filler mass concentrations. Two basic dielectric quantities are measured: amplitude of electrical conductivity (Y) and delay angle (ϕ). These results were compared with the electrical response of parallel RC circuits. Dielectric responses of composites, measured by applying sine and triangle voltage waveforms, differ and that difference in some way is similar to a difference obtained by numerical simulation of parallel RC circuit. The results are showing that by comparing dielectric quantities measured by sinusoidal and triangle signals can get more information about physical parameters which define electrical behavior of polymers and polymer composites. This material and composites at all are interesting in aspect of wide field of application in electronics and open new field for research.

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TM 44

POLY(METHACRYLIC ACID)/ZEOLITE HYDROGEL COMPOSITES AS ADSORBENTS FOR CATIONIC DYE REMOVAL

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Hydrogel composites based on poly(methacrylic acid) and two types of zeolite, zeolite A and zeolite ZSM-5, have been synthesized, characterized by FTIR and SEM analysis and their adsorption potentials toward model cationic dye, Basic Yellow 28, have been investigated under various experimental conditions. Adsorption kinetics and equilibrium studies were performed by batch technique. Adsorption capacities showed to be highly sensitive to change of the initial dye concentration, solution pH, sorbent mass and temperature, as well as zeolite concentration, much more than zeolite type. Image analysis proved to be useful method for analysis of uniformity of coloration along the hydrogel diameter.

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TM 45

SYNTHESIS OF POLYSTYRENE-*G*-STARCH COPOLYMERS USING NEW INITIATOR/*CO*-INITIATOR SYSTEM

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Potassium persulfate (PPS)/different aminewas the new initiator/*co*-initiator system for synthesis of PS-*g*-starch copolymers. Propyl-, iso-butyl-, pentyl-, hexyl-, triethylamine, *N,N*-dimethyl- and *N,N*-diethylethanolamine, 1-(2-hidroxyethyl) piperazine and 4-(2-hidroxyethyl) morpholine were used with aim to obtain graft copolymers with the highest percentage of grafting. All amines, except*N,N*-diethylethanolamineand piperzine derivate, shown activator influence on polymerization reaction. Maximal obtained percentage of grafting was doubled compared with system without amine (32.55 % with *N,N*-dimethylethanolaminecompared to 16.24 %). Copolymers were characterized with FTIR spectroscopy and SEM microscopy. PPS/amines were better systems for initiation than PPS, which was confirmed by higher percentage of grafting.

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TM 46

A SURVEY OF GRP PIPES DEFECTS AND DAMAGE DUE TO FABRICATION PROCESSES

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Glass Reinforced Plastics, commonly known by various standards, as Fiber Reinforced Plastics (FRP), GRP, Glass Fiber Reinforced Plastic (GFRP), Reinforced Plastic Mortar Pipe (RPMP) or Reinforced Thermo-set Resin Plastic (RTRP) is an amalgamation of resin, glass fiber, manufactured using appropriate additives and treatment methods. It is a composite engineering material uniquely capable of meeting a wide variety of specific processes and end product requirements of various applications of fluid transport requirements. GRP piping system is often utilized in almost all applications to withstand aggressive service, ambient and environmental conditions. It has been successfully used in various piping systems and applications over the entire world. GRP piping industry in Libya has just started (i.e. since 2009), so such manufacturing plants are facing some difficulties during commissioning and production trails stage. GRP piping industry has wide variations both in designs and manufacturing techniques used. This paper will focuses and discuss the possible defects associated with the production of GRP pipes, from the point of view of human error, and or lower manufacturing skinless due to new technology introduction in the area. The survey will involve and demonstrate the usage of GRP for various aggressive fluids and its consequences. Finally, concluding remarks concerning defect types, causes, and the prevention of such defects will be presented.

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Y 1

INVESTIGATION OF THE STRUCTURE OF NANOSIZED Na_nCl_n (n = 8, 16, 24, 32) CLUSTERS USING GLOBAL OPTIMIZATION

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The structure and stability of alkali halide clusters has long been a focus of research in an effort to understand crystal growth. In our study, several global optimization methods have been applied to locate both the global and metastable minima of Na_nCl_n (n = 8, 16, 24, 32) clusters. The global search methods using empirical potentials consisted of both simulated annealing (SA) and multiquench (MQ), for comparison, where both single and multi-atom moves were used to generate new atom configurations. For simulated annealing, different temperature schedules, initial temperatures and stopping criteria were applied, while for the multiquench algorithm the number of random walks, number of quenches and the initial temperatures were varied. Furthermore, we used four different types of moveclasses, varying the percentage of single and multi-atom moves. For the larger clusters (n = 24, 32), the multiquench method found an average lower energy minima than simulated annealing. The most relevant lowest-energy structures for the Na_nCl_n clusters are visualized and analysed with the structure drawing and analysis program KPLOT, where we analyze the degree to which the clusters found resemble cut-outs of bulk NaCl.

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Y 2

ELECTRICAL PROPERTIES OF MULTIDOPED CERIA

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Ceria ceramics were obtained from multidoped nano sized ceria powders prepared by both modified glycine nitrate procedure (MGNP) and self - propagating reaction at room temperature (SPRT). Oxides of rare earth elements such as Nd, Sm, Gd, Dy, Y were used as dopants in constant range of 20 %. Samples were sintered at 1500 °C for 1 h in an air atmosphere. XRPD, SEM and electrochemical impedance spectroscopy (EIS) measurements were carried out on sintered samples. It was found that single - phase was formed for each of the sintered materials. The values of conductivity at 700 ^{o}C are higher for the SPRT sample than for MGNP, 2.19×10^{-2} and 1.40×10^{-2} Scm^{-1}, respectively.

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Y 3

DOPED WITH Cu AND Mn ZINC OXIDE CATALYSTS FOR OXIDATION OF Co IN NOXIOUS EMISSIONS

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Quick pace of growth of energetics and chemical industry conduct to sharp contamination of the air, the water and the soil. The presence in the air of noxious emissions from CO, NO, H_2S and hydrocarbons from internal-combustion engines and from the industry is a serious ecological problem. Innovative technology for decrease of the air contamination is the catalytic disposal. Carbon monoxide can be removed using catalytic complete oxidation, which is achieved with catalysts possessing high effectiveness and stability on variable thermodynamic conditions. Supported catalysts, using Pt active component or catalysts with high content of oxides of 3d transition metals are widespread for decontamination of waste gases. There is a great interest in recent catalyst synthesis technologies related to low percentage catalysts with active phase Cu and Mn on supporting precursor. The choice of precursor for the active component and for the basic composite appears as important problem. In the recent work doped with Cu and Mn zinc oxide is investigated as catalyst for oxidation of CO. The pure ZnO and the doped with Cu and Mn zinc oxide samples are synthesized from carbonate, acetate and nitrate precursors. The content of Mn and Cu in the catalyst compositions is less than 1 wt%. For structural, textural and morphological characterization of the samples trivial methods were used: AAS analysis, X-ray Diffraction, BET, EPR, XPS, IR as well as measurements of catalytic activity. The results from recent investigation show high perspective for the catalysts, synthesized from carbonate precursors.

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Y 4

MINIMAL REQUIRED WALL THICKNESS COMPARATIVE ANALYSIS OF A STABLE TANK MADE OF STAINLESS STEEL WITH AND WITHOUT STRAIN HARDENING

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Minimal required wall thickness calculation of a stable horizontal tank, intended for storage of cryogenic gases, made of austenitic stainless steel X5CrNi 18-10 was performed. Tank wall thickness calculation is done in the case of both, strain hardened and non-treated materials. The strain hardened austenitic stainless steel X5CrNi 18-10 achieves significant quantity material savings. Also, the application of strain hardened steel for making tankers, besides savings in materials, increase energy efficiency.

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Y 5

REDUCING THE PARTICLE SIZE OF Bi_20_3 AND Fe_20_3 FOR THE SYNTHESIS OF $BiFeO_3$

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For the synthesis of $BiFeO_3$ from a Bi_2O_3-Fe_2O_3 mixture it is necessary to reduce the particle size to promote the reaction between initial powders. The aim of this work was therefore to obtain a reduced particle size of the initial Bi_2O_3 and Fe_2O_3 powders. For this purpose, we used ball milling in a planetary mill. We analyzed the particles size using granulometric analysis and scanning electron microscopy (SEM). The phase composition of the sintered samples was determined by x-ray diffraction (XRD) analysis. The powders behavior was characterized by TG/DTA and Heating stage microscope.

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Y 6

COMPARATIVE ANALYSIS OF CESIUM SORPTION BEHAVIOR OF THERMALLY, MECHANO-CHEMICALLY MODIFIED AND RAW DIATOMITE

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This paper presents the effect of cesium immobilization in raw and modified diatomaceous earth (DE). The modification of diatomite was carried out by mixing DE and Ti powder mechano-chemically and thermally. X-ray diffraction (XRD) of samples modified by different way was performed. Thermal processing leads to structural changes of diatomite. The specific surface of diatomite which is available for the immobilization of cesium is modified by mechano-chemical treatment for different time. The effect of cesium immobilization of diatomite increases after mechano-chemical treatment, especially for 22h.

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Y 7

ELECTRON SPIN RESONANCE STUDY OF GAMMA-IRRADIATED PLLA

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In order to examine the influence of the initial preparation conditions on the evolution of free radicals in gamma irradiated PLLA, the samples with a large variation in crystallinity were prepared and exposed to gamma radiation, in air, to various absorbed doses (up to 100 kGy). The presence and evolution of free radicals were followed using ESR spectroscopy for three weeks. In addition, SEM, DSC and WAXD measurements were performed. Presented results show that depending on the initial preparation conditions, the radiation-induced changes in structure and properties of PLLA, as well as the evolution of free radicals, can differ significantly.

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Y 8

ADSORPTION OF ARSENIC(III) FROM AQUEOUS SOLUTIONS ON CARBON CRYOGEL

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Arsenic (III) removal from aqueous solutions using carbon cryogel (CC) as adsorbent is presented in this work. CC was obtained by pyrolyzing resorcinol-formaldehyde cryogels in an inert atmosphere. Characterization by nitrogen adsorption showed that the CC was micro and mesoporous materials with high specific surface areas. The adsorption of arsenic (III) on CC was studied as a function of arsenic concentrations, as well as a function of solution pH. Kinetic and equilibrium studies were performed.

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Y 9

THE EFFECT OF CHEMICAL COMPOSITION ON SWELLING AND MECHANICAL PROPERTIES OF P(HEMA/IA/OEGA) HYDROGELS

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In order to investigate the influence of mole fractions of IA and OEGA on swelling properties of the P(HEMA/IA/OEGA) hydrogels, a series of hydrogels with different mole ratios of monomers was synthesised by gamma radiation. The hydrogels were characterised by swelling studies in wide pH and temperature range, confirming pH and thermo responsiveness and a large variation in the swelling capability. In addition, FTIR, SEM, and mechanical measurements were performed, confirming that the properties of hydrogels can be tuned by variation in their composition. Presented results show that the obtained hydrogels can be a beneficial synergetic combination for controlled drug delivery.

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Y 10

NUMERICAL SIMULATION OF ROPEWAY OF AIRLIFT VEHICLES: CALCULATION METHODS

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In first phase of this paper we will briefly give some historical background on the ropeway usage and its importance. Also in this paper we will present the vortex-exited vibration on which we later will create bicable model ropeway via dynamic model. Continuing with these models we will discuss the technical and natural problems that airlift ropeway transportation face. Further we will present the mathematical model using numerical stimulation which satisfies the engineering criteria. Also we will discuss the simulation of load and stresses happening in different stages of air lift operations. The final point for discussion in this paper is the measuring method for chair lifts and bicable ropeways. Calculation for the operation and its validation and maintenance will be made using calculation models such are MBS and ADAMS programs.

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Y 11

LOCAL AND ELECTRONIC STRUCTURE AROUND MANGANESE IN MULTI-COMPONENT SEMICONDUCTORS

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Magnetic ions diluted in semiconductor host make it possible to manipulate spin of electron in addition to its charge, which has a great potential for application of these materials, known as diluted magnetic semiconductors (DMS), in future spintronic devices. This paper presents studies of manganese in multicomponent II-VI and IV-VI semiconductors by means of X-ray Absorption Fine Structure (XAFS). Complemented with the first-principles calculations, these studies provide detailed information on local and electronic structure around manganese ions which is essential for better understanding of magnetic interaction mechanisms in these technologically very important materials.

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Y 12

SURFACE DIELECTRIC RELAXATIONS OF ISOTACTIC POLYPROPYLENE (IPP) AFTER ILLUMINATION AT DIFFERENT TEMPERATURES

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Isotropic iPP sheets were obtained by compression molding at 470 K and pressure of 1.75 MPa, followed by quenching in water at room temperature. Square shaped samples (1x80x80 mm) were cut from the middle of the sheets. For electrodes we have used system of parallel metal wires, which has been hot pressed on the samples surface. Distance between two neighboring wires is 1.5 mm. Dielectrical measurements were performed at 1 kHz before, during and after illumination with visible light at different temperatures ranging from 20 to 50 °C. Prior to the measurements, samples were kept for seven days in the dark. Period of illumination is 10 s. After illumination dielectrical relaxation were recorded for four hours. Consequence of illumination is drop of AC conductivities and relaxation of this process is accelerated with increasing temperature.

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Y 13

SURFACE DIELECTRIC PROPERTIES OF LOW-DENSITY POLYETHYLENE (LDPE) IN VARIABLE VISIBLE LIGHT CONDITIONS

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Isotropic LDPE sheets were obtained by compression molding at 460 K and pressure of 1.75 MPa, followed by quenching in water at room temperature. Square shaped samples (1x80x80 mm) were cut from the middle of the sheets. For electrodes we have used system of parallel metal wires, which has been hot pressed on the samples surface. Distance between two neighboring wires is 1.5 mm. Dielectrical measurements were performed at 1 kHz before, during and after illumination with visible light. Prior the measurements, samples were kept for seven days in the dark. Period of illumination varied between 2 and 100 s. After illumination dielectrical relaxation were recorded for two hours. Since the samples were kept in the dark, illumination triggered the drop in electrical conductivities. This effect can be explained with formation of electron curtain around metal wires.

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Y 14

NEW FACILE SYNTHESIS ROUTE FOR OBTAINING PHASE PURE $LiFePO_4$/C COMPOSITE

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Carbon-coated, olivine-structured $LiFePO_4$ suitable for cathode material in rechargeable lithium batteries has been prepared via simple, both time and energy low-consuming synthesis route. Procedure involves soaking of cellulose-containing substrate with aqueous precursor solution followed by rapid (several minutes long) single heating step. Cellulose acts as (i) reducing agent and (ii) carbon source which suppresses growth and prevents agglomeration of $LiFePO_4$ particles and also creates a conductive network in $LiFePO_4$/C composite. The crystalline structure, morphology and charge/discharge performance of the as-prepared composite were investigated by means of XRD analysis, electron microscopy and galvanostatic charge-discharge tests. $LiFePO_4$/C powder appears to be nanocrystalline (with mean crystallite size of 37 nm) and electrochemically stable achieving 97% (165 $mAhg^{-1}$) of its theoretical capacity.

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Y 15

BIOACTIVE COMPOSITE MATERIALS IN REGENERATION OF THE RESORBED BONE OF ALVEOLAR RIDGES

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Bone loss during the systemic osteoporosis has an important role in dentistry and medicine. The aim of the study was the application of bioactive micro-and nano-composite materials, alone, and in combination with autologous plasma in osteoporotic jaw bones of rats with artificially induced osteoporosis. The effect of these composites was measured by histomorphometric and atomic absorption spectrophotometric analysis. According to the best obtained results in regeneration and recovery of the resorbed alveolar bone, it can be concluded that nano-composite combined with autologous plasma may be the material of choice to replace the osteoporotic damaged jaw bone.

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Y 16

EFFECTS OF DIFFERENT CRYOPROTECTANTS ON MORPHOLOGY OF LYOPHILIZED POLY(ε-CAPROLACTONE) MICRO- AND NANOSPHERES

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A common limitation of using polymeric micro- and nanoparticles in long-term conservation is due to their poor physical and chemical stability. Freeze-drying is one of the most convenient methods that enables further reconstitution of micro- and nanoparticles for therapeutical use. Nevertheless, this process generates various stresses during freezing and desiccation steps. The aim of this study was to evaluate different cryoprotectants (protective excipients that are usually added to increase stability upon storage and protect the particles from freezing stress): sugars (glucose and sucrose) and polymers (PVA and PGA), on the outcome of freeze-dried poly(ε-caprolactone) micro- and nanospheres. The best freeze-drying results in terms of morphological characteristics, analized with SEM, were achieved with glucose at concentration of 1%. The FT-IR analysis confirmed that the molecular structure of PCL particles remained the same after the addition cryoprotectants.

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Y 17

SYNTHESIS AND CHARACTERIZATION OF SELENIUM NANOPARTICLES IN THE PRESENCE OF BOVINE SERUM ALBUMIN OR POLY (L-GLUTAMIC ACID) FOR BIOMEDICAL APPLICATION

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It is well known that selenium is an essential trace element playing the important roles in mammalian biology. For years, its organic forms and some salts have been used in studying its biological effects, but recently, selenium nanoparticles have gained great attention as a possible material for cancer therapy and prevention. In this study we report the facile and reproducible method for synthesis the nano-selenium by reduction of sodium selenite with an ascorbic acid, in the presence of a two stabilizing agents, bovine serum albumin (BSA) or poly (L-glutamic acid) (PGA). The influence of the sodium selenite/ascorbic acid ratio as well as the types and concentration of two different stabilizers on the wide variety physicochemical characteristics of obtained particles were examined.

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Y 18

THE EFFECT OF AGING OF MILLED CLAY ON THE REMOVAL EFFICIENCIES OF HEAVY METAL IONS

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The influence of aging on sorption behavior of natural clay modified by mechanical milling for different milling periods has been investigated. The changes in microstructure of samples investigated by PSD and XRD analysis were correlated with adsorption properties. Aging affects the removal efficiencies of the heavy metal ions (Pb(II), Cd(II), Cu(II), Zn(II)) from aqueous solutions. The best removal efficiencies as function of time of aging show sample milled 19h in comparison with samples milled 1 h, 2 h and 10 h. This behavior is related to the re-crystallization of the amorphizated 19h milled sample.

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Y 19

DRUG DELIVERY PARADIGM OF SILVER IONS RELEASED FROM AG/PVA HYDROGEL NANOCOMPOSITES OBTAINED BY RADIATION CHEMISTRY NANOREACTOR METHOD

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The importance of silver ion in the biological response to nano-silver is widely recognized hence there is significant potential to improve nano-silver technologies through controlled release formulations. In this study, kinetic analysis of silver ion release of γ-radiolytically synthesized Ag/PVA hydrogel nanocomposites was performed. Different model fitting methods were applied to estimate kinetic parameters. The analysis showed that the curvilinear nature of the cumulative percent silver released versus time provides the closest fit between experimental observations and the nonlinear function. The investigation of antimicrobial properties indicate that the size of Ag nanoparticles beside their molar concentration, have meaningful importance for antibacterial activity.

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Y 20

SWELLING STUDIES OF THERMO- AND pH-SENSITIVE Ag-POLY(NiPAAm/IA) HYDROGEL NANOCOMPOSITES SYNTHESIZED BY GAMMA IRRADIATION

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This work describes radiation-chemical induced *in situ* incorporation of silver nanoparticles (Ag NPs) within poly(NiPAAm/IA) hydrogels, previously crosslinked also by gamma irradiation, in order to obtained hydrogel nanocomposites. The formation of Ag NPs was confirmed by appearance of characteristic surface plasmon absorption band at around 400 nm, while their average size was determined by Mie's theory. The physico-chemical properties of pure and nanocomposite polymer networks were investigated by swelling measurement under the different condition. Obtained results showed that amount of IA have strong influence on swelling and diffusion properties of hydrogels, whereas the influence of Ag NPs is almost negligible.

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Y 21

KINETIC STUDY OF PALLADIUM SORPTION BY MACROPOROUS COPOLYMER

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Palladium is widely used in electronics, medicine and catalysis due its corrosion and oxidation resistance, electrical conductivity and catalytic activity. Because of high cost and low availability, the separation and recovery of palladium rises as important issue. In this study, the possibility of Pd ions recovery from aqueous solutions by macroporous poly(glycidyl methacrylate-*co*-ethylene glycol dimethacrylate) with attached diethylene triamine (PGME-deta) from acidic medium (pH 2) at 298 K was investigated. Four kinetic models were evaluated in order to understand the mechanism of palladium (II) sorption. The concentration of Pd(II) ions was measured by inductively coupled plasma optical emission spectroscopy (ICP-OES).

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Y 22

EXAMINATION OF THE INFLUENCE OF NANOMATERIALS CALCIUM PHOSPHATE/POLY-(DL-LACTIDE-CO-GLYCOLIDE) AND COBALT-EXCHANGED HYDROXYAPATITE ON THE VIABILITY OF SAOS-2 CELLS

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We have examined the effect of extracts of the calcium phosphate/poly-(DL-lactide-co-glycolide) (CP/PLGA) and cobalt-exchanged hydroxyapatite (CoHAp), on the viability of Saos-2 osteoblast-like cells. Extracts were prepared by incubation for 3 days at 37^0C in the cultivation medium. Conductivity and pH value of extracts were measured before viability assay. Cell viability was estimated by MTT test performed after 24 h incubation of cells with various concentrations of extracts. Extract of CP/PLGA acted more cytotoxic on osteoblasts than the extract of CoHAp. This difference in the effect of examined extracts can be explained by their different pH value and conductivity.

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TH 1

POLYMORPHISM AND STABILITY OF MAGNESIUM BOROHYDRIDE

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In order to understand stability and structural properties of magnesium borohydride, we studied, by synchrotron powder diffraction, temperature-induced transformation of its hexagonal α- and cubic γ-polymorphs, both under vacuum and hydrogen back-pressure. The decomposition pathways depend strongly on the experimental conditions. Under vacuum, γ -phase first turns into the β-phase, which further evolves into a related structure, hereafter called β '. α-$Mg(BH_4)_2$ under vacuum transforms into a new polymorph, called here ε. As a number of $Mg(BH_4)_2$ polymorphs resemble SiO_2 structures, the database of observed/predicted SiO_2 frameworks can help to identify new $Mg(BH_4)_2$ structures.

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TH 2

ACHIEVING HIGH CAPACITY REVERSIBLE HYDROGEN STORAGE: $NaBH_4$@Ni CORE-SHELL NANOPARTICLES

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Sodium borohydride ($NaBH_4$) is a promising on-board hydrogen storage material. This research aimed to pioneer high capacity reversible storage under reasonable conditions. Nanoprecipitation allowed synthesis of nano-$NaBH_4$, with some improvements but no reversibility. Nanoconfinement via a core-shell approach, $NaBH_4$@Ni, provided an effective strategy to contain the melted $NaBH_4$ core and its dehydrogenation products, preventing their dispersion. At 350 °C, a steady reversible capacity of 5 mass % was achieved with fast kinetics. Under a heating ramp hydrogen release began at only 60 °C. This strategy has great potential for major advancements in the design of effective hydrogen storage materials.

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TH 3

HYDRAZINE BORANE AND DERIVATIVES AS CHEMICAL HYDROGEN STORAGE MATERIALS

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Hydrazine borane $N_2H_4BH_3$ has been recently presented as being a derivative of ammonia borane NH_3BH_3 with a potential in chemical hydrogen storage. Involved in this reserach field, we optimized the synthesis of this new material and establishedacomplete data sheet (NMR, IR, XRD, TGA and DSC). However, under heating, it releasessignificantamount of pure hydrazine and leads to the formation of a shock-sensitive solid residue, which make it unsuitable for application. Hence, we intensified our works on synthesizing derivatives, and we successfully prepared and characterized (NMR, IR, XRD, TGA and DSC) two different and novel (never-reported heretofore) materials. Both showed improved dehydrogenation properties while not displaying the drawbacks of their parent. Our last results will be presented during the "*the 1st European Early Stage Researcher's Conference on Hydrogen Storage*".

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TH 4

PHYSICAL AND CHEMICAL PROPERTIES OF VOLATILE COMPLEX HYDRIDES

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The storage of hydrogen in liquid complex hydrides is an attractive option. However, difficulties in their characterization are a matter of fact, with particular emphasis on their gaseous products. The presented investigation method uses a thermogravimetric balance to monitor the sample weight loss, while the decomposition gas is detected by an infrared spectrometer. We investigate metasynthesis of Ti(BH4)3 and Al(BH4)3. It is shown that the analysis of the gas phase is fundamental in order to understand their decomposition reactions: these materials emit hydrogen containing volatile species, such as diborane, which is an issue for their reversibility.

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TH 5

AMMONIA BORANE NANOCONFINEMENT INTO CARBONACEOUS OR BORON-NITROGEN-BASED HOST MATERIALS

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Ammonia borane NH_3BH_3 is considered as the most promising chemical hydrogen storage material since the mid 2000s owing to its ability to liberate dihydrogen under heating. However, the 13 wt% H can be released only over the range 100-200 °C. To decrease these temperatures as well as to improve the purity of H_2, one of the strategies we have adopted is to confine NH_3BH_3(in tetrahydrofuran solution) into meso- and micro-porous hosts such as activated carbon or boron nitride. The as-formed composites were analyzed by ^{11}B MAS NMR, IR, XRD, TGA and DSC. One of the striking results is that NH_3BH_3 nanoconfined into activated carbon released dihydrogen in room conditions owing to acid-based reactions. Our last results will be presented during the "*the 1st European Early Stage Researcher's Conference on Hydrogen Storage*

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TH 6

THE EFFECTS OF Si AND EXPANDED PTFE SUBSTRATES ON FORMATION AND HYDROGENATION OF Mg AND Mg-Ti FILMS

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Usually metallic films for metal hydrides research are deposited on hard and flat substrates such as silicon, magnesium oxide etc. With the film thickness increases all films during hydrogenation deals with typical problems such as film brittleness and cracking. In this paper we demonstrate that metal Mg and Mg-Ti films for hydride formation can be successfully deposited on the flexible Expanded PTFE substrates. The received results for ePTFE substrates are compared to the films being deposited on Si with different plasma pretreatment. It is discussed that different interface properties between substrate and film can have effect on film morphology, crystallinity and its reaction with hydrogen.

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TH 7

METAL HYDRIDE FILMS FOR OPTO-ELECTRONIC APPLICATIONS

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Metal hydrides cannot only reversibly store hydrogen: they can also be applied as active materials in thin-film electrical and optical devices. A number of metal-hydride materials have been investigated for such purposes. This talk will give an overview of advances with respect opto-electronic applications of thin-film metal hydrides. Such applications comprise technologies as smart windows, hydrogen sensors and potentially photovoltiacs. I will go through relevant recent research results by our group: a study of the semiconducting properties of Mg-Ni hydride films and the recent discovery of a strong photochromic effect in films of yttrium hydride.

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TH 8

LASER SURFACE MODIFICATION OF MATERIALS

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A series of alloys (H13 tool steel, 316 stainless steel, Ti-6Al-4V) and WC-CoCr coating surface were modified by a 1.5 kW CO_2laser in both pulsed and continuous mode in a high speed sample processing condition. Several design of experiments (DoE) were carried out to optimize the laser processing parameters which include, peak power, spot diameter, pulse repetition frequence, irradiance etc. The effect of laser processing parameters on the microstructure, surface roughness, melt pool depth, phase transformation, residual strain, microhardness, and chemical composition were investigated. In most cases, laser surface modification has resulted in better surface properties of materials.

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TH 9

MODIFICATIONS IN MICROSTRUCTURE OF MgH_2-BASED COMPOSITE UPON HYDROGEN CYCLING

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Kinetics modifications upon hydrogen cycling of composite materials obtained by ball milling MgH_2 with different additives were studied by the mean of a Sievert volumentric Apparatus. The microstructural evolution of the material during a sequence of H_2 sorption cycles was explored by the Scanning Electron Microscopy. Independently of the nature of the additive, the original microstructure of MgH_2 is strongly affected by the cycling procedure. Besides particle coarsening, the presence of material protruding from the particle surface in a worm-like structure is observed. Hollow particles constituted by empty MgO shell box are also noticed.

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TH 10

TUNING THE HYDROGEN STORAGE OF MOFS BY INTRODUCING METALS ON THE LINKER SIDE

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Hydrogen storage is arguably the biggest challenge in developing a hydrogen economy. While different types of materials are being explored as hydrogen carriers, porous materials have the advantage of offering fast kinetics for hydrogen sorption as well as reversibility over multiple cycles. Among them, metal-organic frameworks (MOFs) are being increasingly considered as promising materials for non-dissociative hydrogen adsorption. They display high crystallinity as well as high and regular porosity. In addition, their syntheses can be carried out under mild conditions, allowing for their rational design and facile pre- or post-synthetic modification. Hydrogen-storage capacity of MOFs can either be enhanced by increasing their surface area and pore volume or by increasing the hydrogen's isosteric heat of adsorption. While there are several publications showing that the introduction of metal ions in the pores by cation exchange or doping, it has only been recently suggested that the introduction of cations on the the linker site could also result in an increased hydrogen uptake. However, to date no convincing evidence has been provided for this theory, This work supplies the first data on how metal coordination on the linker site influences the hydrogen-storage properties of metal-organic frameworks. Pd2+ was infused in the pores of NH2-MIL-101 as it specifically bind to the NH2- functional groups. This enables the selective introduction of the Pd2+ on the linker site (as long as the loading remains sufficiently low). Subsequently hydrogen-adsorption data was collected at 77 K and ambient temperatures and the results were compared to those obtained on the pristine NH2-MIL-101 under the same conditions. In the present work, the findings of this comparison, i.e. the effect of the metal infusion on the MOF's linker site will be discussed.

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TH 11

SYNTHESIS AND HYDROGENATION OF $Mg_6Pd_{1-x}TM_x$ (TM =Ag, Cu) NOVEL SYSTEMS

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Mg_6Pd intermetallic compound has been actively investigated as a hydrogen storage material. Substituting Pd by other transition metals can destabilize the hydride and reduce the cost of the alloy. $Mg_6Pd_{0.5}TM_{0.5}$ (TM = Ag, Cu) samples have been synthesized by induction melting. Scanning Electron Microscopy analysis, X-ray powder diffraction and Electron Probe Micro-Analysis were used to determine phase composition and abundance. Cu solubility in Mg_6Pd is limited to x = 0.3. For the Ag containing sample the ternary phase $Mg_{5.8}Pd_{0.7}Ag_{0.5}$ is formed. This one reversibly absorbs up to 3.1 wt.% H, decomposing into MgH_2, Mg_5Pd_2 and MgPd phases, with Ag partially substituting Pd atoms. Both systems have been investigated by High Pressure Differential Scanning Calorimetry. Several (endo-) exothermic peaks are observed, indicating that (de-)hydrogenation occurs in several steps. The mechanisms involved during hydrogenation process will be discussed.

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TH 12

STRUCTURE AND HYDROGEN STORAGE PROPERTIES OF THE HEXAGONAL LAVES PHASE $Sc(Al_{1-X}Ni_X)_2$

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The crystal structures of hydrogenated and unhydrogenated $Sc(Al_{1-x}Ni_x)_2$ Laves phases have been determined by combining several diffraction techniques and it is shown that hydrogen is situated interstitially in the A_2B_2-site, which has the maximum number of scandium neighbours. The hydrogen absorption/desorption behaviour has also been investigated. It is shown that hydrogen absorption forms a solid solution of hydrogen in the mother compound. The hydrogen storage capacity exceeds 1.7 H/f.u. at 374 K. The activation energy of hydrogen desorption was determined to 4.6 kJ/mol H_2.

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TH 13

MICROSTRUCTURE EVOLUTION IN THE CHIPS OF MG-10 AT.% NI ALLOY DURING HYDROGENATION

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The aim of the study was to establish the correlation between hydrogenation properties and microstructure of hypoeutectic Mg-10 at.% Ni alloy in the as-cast state and after processing by equal channel angular pressing (ECAP). The initial microstructures of as-cast and ECAP-processed alloys are quite similar, but intermittent hydrogenation behavior is very different. It was found that hydrogenation promotes growth of large faceted Mg single crystals in the chips of both alloys. Although a significant morphological difference between the chips of as-cast and ECAP-processed alloys was observed during initial hydrogenation cycles, after nine cycles the morphology and hydrogenation kinetics of both samples become nearly identical.

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TH 14

COMBINATORIAL SYNTHESIS AND HIGH THROUGHPUT EXAMINATION OF HYDROGEN STORAGE ALLOY LIBRARIES

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Binary and ternary alloy libraries (from Fe-Ti and Fe-Ti-Ni systems) were synthesized by Laser Engineered Net Shaping technique. Discrete and continuous micro-libraries as well as large in-situ alloyed samples were prepared in a course of one experiment. Chemical composition examination, X-Ray phase analysis have shown that synthesis was performed with success. Fe-Ti and Fe-Ti-Ni samples absorbed significant amounts of hydrogen close to theoretical without any complication activation. New method for high throughput examination of hydrogen storage properties based on custom made multi-Temperature Programmed Desorption device is presented.

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TH 15

STRUCTURAL CHARACTERIZATION AND ELECTROCHEMICAL HYDROGEN STORAGE PROPERTIES OF Ti2Ni AND $(Ti1\text{-}xZrx)_2Ni$ (x=0, 0.05, 0.1) ALLOYS PREPARED BY MECHANICAL ALLOYING

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Nominal Ti2Ni were synthesized by ball milling. The effect of milling time on the characteristic and hydrogen performance was investigated. Amorphous phase was obtained after 60 hours of milling, which showed the best hydrogen performance. The sample containing mainly amorphous phase had stable discharge capacity at about 100mAh/g under room temperature without the need of activation. Zr substitution for Ti was also introduced to the 60h milling time Ti2Ni powder with a formula (Ti1-xZrx)2Ni (x=0, 0.05, 0.1). It is found that Zr hindered amorphization process and increased the MT temperature of Ti-Ni system, thus an austenitic crystal structure was formed, which had steady but poor hydrogen discharge capacity under room temperature.

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TH 16

COMPUTATIONAL SCREENING OF MIXED METAL HALIDE AMMINES

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Metal halide ammines, e.g. $Mg(NH_3)_6Cl_2$ and $Sr(NH_3)_8Cl_2$, can reversibly store ammonia, with high volumetric hydrogen storage capacities. In this project we are searching for improved mixed materials with optimal desorption temperature and kinetics. We apply DFT calculations on mixed compounds selected by a Genetic Algorithm (GA), relying on biological principles of natural selection. The GA is evolving from an initial (random) population and selecting those with highest fitness, e.g. stability, release temperature and storage capacity. The search space includes all alkaline, alkaline earth, 3d and 4d metals and the four lightest halides, giving in total almost two million combinations.

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TH 17

INVESTIGATION OF SURFACE AND NEAR-SURFACE EFFECTS ON HYDROGEN DESORPTION PROPERTIES OF MgH_2

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In attempt to comprehend and improve desorption behaviour of MgH_2 we have investigated the influence of structural changes introduced by ion irradiation into MgH_2 matrix. The changes were followed by both, experiment and theory using XRD, particle size analysis, TPD and Ab initio calculations. Results suggest that there are several mechanisms involved in desorption process, which depend on defect concentration and their interaction and ordering. It has been demonstrated that the changes in near-surface area play the crucial role in desorption kinetics. It is also confirmed that there is possibility to control the thermodynamic parameters by controlling vacancies concentration.

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TH 18

COMPUTATONAL STUDY OF H STORAGE IN Pd AND Pt NANOPARTCICLES SUPPORTED ON MgO

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The hydrogen storage properties of Pd are well known and could be improved by its nanostructuring. There is experimental evidence that Pt nanoparticles are also able to absorb hydrogen, in contrast with bulky Pt samples. In this work we investigate H adsorption and absorption at low and high coverage on scalable to bulk Pd and Pt nanoparticles supported on MgO(100) using density functional methods. It is found that high H surface coverage promotes H absorption into the bulk sites and makes this process feasible on Pd nanoparticles, but in the case of calculated Pt nanoparticles H absorption remains highly endothermic.

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TH 19

HYDROGEN STORAGE PROPERTIES OF SUMANENE

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Hydrogen is concerned as an ideal energy carrier and ideal energy source for replacement of limited and harmful fossil fuels. Adsorbents of hydrogen have to have large surface areas and suitable binding energies. It is important to obtain intermediate binding energies between H_2 and adsorbing structure since these energies allow both adsorption and release. These conditions are reached by nanotubes and fullerenes, and, according to our work, by sumanene as well.
We investigated adsorption properties of sumanene towards H_2 using density functional theory computations. Investigation encompassed study of MEP surfaces, quantum molecular descriptors, NMR parameters, NICS, NBO/NPA analysis and DOS.

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TH 20

STRUCTURAL AND HYDROGEN SORPTION PROPERTIES OF $SmNi_{5-x}Ga_x$ SYSTEM – AN EXPERIMENTAL AND THEORETICAL STUDY

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A series of ternary alloys of general formula $SmNi_{5-x}Ga_x$ was prepared by melting stoichiometric mixtures of Sm, Ni and Ga in arc furnace under argon. From X-ray powder diffraction lattice parameters are determined and it is found that hexagonal structure of $SmNi_5$ ($CaCu_5$ type) is retained for all considered values of *x*. Hydrogen absorption ability and thermodynamic quantities of the systems are determined by pressure-composition desorption isotherms. The obtained properties are compared with those of previously reported $SmNi_5$ and $SmNi_4Ga$. DFT calculations were performed for selected members of the system and the results are discussed with regard to experiment.

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TH 21

INDUCTION PLASMA SYNTHESIS OF Mg_2Ni NANOPARTICLES FOR HYDROGEN STORAGE

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Mg_2Ni is a well-known alloy that could store 3.6 wt.% hydrogen. Efforts to reduce the stability of this alloy mainly involved compositional alterations as well as reduction in the structural scale with such methods as mechanical milling or thin film deposition. In the present study, Mg_2Ni nanoparticles were synthesized in RF inductively coupled plasma with a nanopowder reactor. Conventional approach of feeding the prealloyed powder into the torch has resulted in disintegration of the intermetallic alloy, producing Mg and Ni nanopowders with a small fraction of targeted Mg_2Ni nanoparticles. As an alternative approach, the prealloyed powders were fed into the plasma from the bottom injector where the Mg_2Ni yield was slightly higher. Feeding the starting material in the form of elemental powders, Ni from the top and Mg from the bottom injector has yielded nanopowders <100 nm in size, where Mg_2Ni had a significant proportion. PCT isotherms of the synthesized nanopowders are being studied currently by a Sievert's type apparatus.

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TH 22

POLYANIONIC GALLIUM-HYDROGEN CLUSTER IONS AS POSSIBLE INTERMEDIATES IN DEHYDROGENATION REACTIONS

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$LiBH_4$ and $NaAlH_4$ have been regarded as promising hydrogen storage materials since both contain a high gravimetric content of hydrogen. The major challenge is the poor kinetics of hydrogen release, hence much research effort has been put in to enhance the dehydrogenation reactions. The cluster ions $[Ga(GaH_3)_4]^{5-}$, $[Ga_nH_{2n}]^{n-}$ and $[Ga_3H_8]^{3-}$ are formed in the air sensitive compounds $Rb_8Ga_5H_{15}$, $AGaH_2$ (A=K, Rb) and $Cs_{10}Ga_9H_{25}$ respectively by exposing a melt of alkali metals (K, Rb, Cs) and gallium to hydrogen gas at elevated temperatures. These compounds represent a new group of compounds featuring polyanionic gallium hydrogen clusters that may serve as intermediates in dehydrogenation reactions for the compounds mentioned above.

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TH 23

EFFECT OF A $CaF_{2-x}H_x$ SOLID SOLUTION FORMATION IN THE MIXED SYSTEM CaH_2+CaF_2 +MgB_2

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In this work the effect of a partial replacement of CaH_2 by CaF_2 on the sorption properties of the system CaH_2 + MgB_2 was studied. The first five hydrogen absorption and four desorption reactions of the CaH_2+MgB_2 and the $3CaH_2$+CaF_2+$4MgB_2$ systems were investigated by means of volumetric measurements, High Pressure Differential Scanning Calorimetric technique, MAS NMR analysis and in situ Synchrotron Radiation Powder X-ray diffraction. It was observed that already during the mixing of the reactants, the formation of a non-stoichiometric $CaF_{2-x}H_x$ solid solution takes place. The formation of the $CaF_{2-x}H_x$ solid solution sensibly affects the overall hydrogen sorption reactions of the system CaH_2 + MgB_2.

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TH 24

DESIGN, SIMULATION AND OPTIMISATION OF AN ANODE SUPPORTED SOFC

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Solid oxide fuel cell is one the technologies that has the potential to be leading the market in the race of clean energies. The first aspect of this research is the production of a sample fuel cell using the most common methods of powder compression and screen printing. The test cell is made using powders of the materials and then sintered in a furnace before other layers are added to complete the cell. The second aspect is the validation of a simulation model using the experimental data available from a commercialised fuel cell. The results of the simulation were validated by comparison between the experimental data. These results suggest a maximum theoretical power density of 0.41 W/cm^2 for the designed cell.

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TH 25

HYDROGEN STORAGE IN POROUS MEDIA AT ROOM TEMPERATURE

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The main aim of this work is to find a porous material that is able to store hydrogen at room temperature and at pressure range from 1 to 10 bars. In our research activated natural zeolite samples are used. Activation of the samples is carried out in ion-exchange process and in pyrolysis process. As the result of the activation the samples were coated by palladium nanoparticles. Amount of stored hydrogen in the samples is determined by thermogravimetric and volumetric methods. The results show that the hydrogen sorption capacity of the coated material is greater than for zeolite or Pd separately.

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TH 26

ENHANCING THE HYDROGEN CARBON INTERACTION

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Carbon is an easily available, light weight and abundant element, able to store large quantities of hydrogen. Covalently bound hydrogen, as in conventionally used hydrocarbons, is inconvenient for hydrogen access due to either high activation or binding energies. For physisorbed molecular hydrogen on high specific surface area carbonaceous materials the binding energy is low and cryogenic temperatures are required for storage. An increased, intermediate, binding energy of 20 – 40 kJ/mol H_2 is desirable and can be achieved by additional attracting forces between the hydrogen molecule and the host material either in the form of electrostatic (dipole or quadrupole) or orbital interaction (Kubas interaction).

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TH 27

HYDROGEN STORAGE PROPERTIES OF DIFFERENT METAL-DOPED CARBON-BASED COMPOSITES

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An interesting approach for the efficient hydrogen solid storage is the use of metal doped carbon materials, where metal nanoparticles (e.g. Pd, Pt) seem to catalytically enhance hydrogen sorption at room temperature on the basis of the so-called spillover mechanism. In the present work we compare the room temperature hydrogen sorption behavior of different Pd-doped carbon-based composites resulting from the combination of various nanostructured carbons (foams, single- and multi- wall carbon nanotubes, fullerenes and graphite) in an attempt to elucidate possible binding sites that may assist the weak chemisorption hydrogen spillover process. Our low pressure (up to 1 bar) hydrogen uptake measurements point to possible intercalation of atomic hydrogen between the graphitic or multi-wall nanotube layers.

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TH 28

PRODUCTION OF SINGLE – WALL CARBON NANOTUBES BY KrF EXCIMER LASER ABLATION

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We report about catalyst influence on carbon single–wall nanotubes (SWNT) synthesis by means of KrF excimer laser ablation of catalyst doped targets prepared by a new technique. The novel target preparation eliminates the need for pressing or hot pressing oh the target. The products have been investigated by high resolution transmission electron microscopy (HRTEM) and Raman spectroscopy. The laser synthesized SWNTs, at a furnace temperature of 1100 ^{0}C, have a narrow diameter distribution. Bundles of SWNTs intertwined with some amorphous carbon species and catalyst particles can be observed in the as-produced SWNTs deposits. The ratio of mixed metallic and semiconducting electronic type of as-grown SWNTs was investigated by means of micro-Raman spectroscopy. The products obtained will be tested in complex systems for their hydrogen storage capacity and other possible applications.

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TH 29

CONFINEMENT OF LIBH4 IN NANOPOROUS CARBON MATERIALS: SIZE AND INTERFACE EFFECTS ON HYDROGEN MOBILITY AND RELEASE

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Lithiumborohydride attracts much attention as a promising material for hydrogen storage (total hydrogen content: 18.5 wt%) but the elevated temperatures required to release the gas are an important obstacle for practical application.In this work we investigate nanosizing effects on decomposition kinetics and we evaluate the limiting factors for hydrogen release. LiBH4 has been confined in different carbon hosts by melt-infiltration; decomposition profiles have been investigated by means of calorimetry, showing a lower dehydrogenation temperature and suggesting a different decomposition pathway than for bulk LiBH4. Surprisingly, nanosizing affects even the LiBH4 solid-solid phase transition temperature and Neutron Scattering and NMR highlighted changes in ion mobility close to interface between LiBH4 and scaffold.

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TH 30

SCANDIUM FUNCTIONALIZED CARBON AEROGELS FOR HYDROGEN STORAGE

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A new nanocomposite material is synthesized for hydrogen storage based on nanoparticles of $NaAlH_4$ melt infiltrated into sc-functionalized carbon aerogel in order to explore possible synergetic effects between nanoconfinement and scaffold functionalization. The scaffold functionalization is utilized by a novel infiltration method, using aqueous $ScCl_3$ as a precursor. Upon drying of the functionalized scaffold, the new compound ScOCl is obtained. Nanoparticles of (5 wt%) ScOCl is residing inside the mesopores of the aerogel, confirmed by HR-STEM and EDS. The kinetic effect of hydrogen release is improved by 3 °C, for the sc-doped scaffold, measured by TPD-MS. During hydrogen release and uptake measured by Sieverts´, the effect induced by melt infiltration into sc-functionalized aerogel leads to a significantly improved reversibility, remaining 62 % of its hydrogen storage capacity, compared to 54 % using pristine aerogel.

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TH 31

DEVELOPMENT OF NOVEL 3D TEM SAMPLE STRUCTURING METHODOLOGIES AND ADVANCED FIB AND TEM TOMOGRAPHY APPLICATIONS FOR NANOPOROUS MATERIALS

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Electron Tomography applications, in particular, are needed for imaging and analysis of ceramic and composite based 3D material systems, such as, hydrogen storage materials, solid oxide fuel cells. This study concerns the development of novel TEM/FIB tomography methodologies to reveal the geometric and chemical distribution of such material systems. In this scope, while the samples to be investigated in the TEM provide 3D information at the nanometer scale and below; via FIB tomography sectioning, the information in the scale ranging from micrometers to tens of nanometers is collected from the identical sample and the data are comparatively and complimentarily evaluated.

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E 1

HYDROGEN SORPTION PROPERTIES OF $MgH_2/NaBH_4$ COMPOSITES

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The hydrogen sorption properties of $MgH_2/NaBH_4$ composites prepared by high energy ball milling under Ar atmosphere were investigated. Samples with different content of $NaBH_4$ and different milling time were prepared. Microstructural and morphological analyses were done by X-Ray Diffraction and Scanning Electron Microscopy. Kinetic analyses and cycling under hydrogen pressure were performed in a Sievert's volumetric apparatus. Results suggest that both low milling time and lower content of $NaBH_4$ have beneficial influence on reactions kinetics and on the amount of sorbed hydrogen.

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E 2

COMBINED SOLID STATE AND HIGH PRESSURE HYDROGEN STORAGE

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The aim is to enable future use of hydrogen as a carrier of renewable energy for transportation that may eliminate particle emissions and fossil fuels dependency. One approach is to combine solid state and high pressure onboard hydrogen storage as this has the potential to increase the storage capacity considerably. The idea is to design chemical reactions that are solely controlled by the pressure and the temperature in the storage tank and are able to absorb both hydrogen and heat. This concept has a potential for fast refueling, high capacity and long driving range.

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E 3

STRUCTURE AND HYDROGEN STORAGE PROPERTIES OF HIGH ENTROPY TiVCrNiFe AND TiVCrNiFeZr ALLOYS SYNTHESIZED BY USING LASER ENGINEERED NET SHAPING (LENS)

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TiVCrNiFe and TiVCrNiFeZr multi-principal-element alloys were fabricated by using the Laser Engineered Net Shaping technique. The influence of the LENS process parameters on the microstructure and hydrogen storage properties of the alloys was studied. The phase analysis was performed with X-ray diffraction. Thereafter, SEM/BSE with EDS mode was used to determine the chemical composition and homogeneity of the alloys. The P-C-T isotherms were measured at 50°C after activation for 2h at 500°C under vacuum. The obtained results showed that alloy with C14 Laves phase structure (FeNiTiCrVZr) are capable of storing relatively large amount of the hydrogen (~1,8% wt.) with rapid absorption/desorption kinetics at room temperature.

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E 4

CHARACTERIZATION OF MULTILAYERED HYDROGEN STORAGE MATERIALS BY TRANSMISSION ELECTRON MICROSCOPY

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Transmission electron microscopy was used to characterize the structure and composition of Si-Fe-Mg-Fe-Pd and Si-Ti-Mg-Ti-Pd multilayered samples that have great interest for hydrogen storage. Both native and hydrogenated states were investigated. High-resolution electron microscopy and electron diffraction were used to derive a structure model for the layers. These results are complimented bychemical characterization done by EDX (Energy Dispersive X-ray Spectroscopy) and EELS (Electron Energy Loss Spectroscopy), which provides additional information regarding layer thickness and intermixing. It was found that the magnesium layer thickness is more consistent in the Si-Ti-Mg-Ti-Pd samples. Also the Mg to MgH_2transition will be discussed.

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E 5

ELECTRONIC STRUCTURE AND FORMATION ENERGIES OF HFV_2H_X LAVES PHASE

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We present calculations of electronic structure, formation enthalpies, and electric field gradients in cubic $HfV_2H_{x=1,2,3,4}$ Laves phase, where hydrogen occupies three interstitial positions, 96g, 32e, and 8b. To determine which one of these interstitials is most favorable for storing hydrogen, formation enthalpies were calculated for every site, while changing x. To investigate electronic structure modifications before and after hydrogenation, we calculated electric field gradients, and compared them with the nuclear magnetic resonance measurements, which enabled us to study the distribution of hydrogen in the crystal lattice, as well as the occupation of interstitials.

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E 6

STRUCTURAL AND ELECTRONIC FACTORS GOVERNING HYDROGEN STORAGE PROPERTIES OF TMNi COMPOUNDS (TM=Ti, Zr, Hf)

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Hydrides of binary and ternary compounds formed between IVb group transition metals and nickel are studied using the full potential (L)APW+lo method within DFT. Differences in hydride formation behavior between ZrNi, HfNi and TiNi are addressed from structural and electronic point of view. Also, electronic structure, bonding and thermodynamical parameters of ternary compound $Ti_{0.64}Zr_{0.36}Ni$ and appropriate orthorhombic hydride are investigated. Contrary to TiNiH, $Ti_{0.64}Zr_{0.36}NiH$ is found to be thermodynamically favorable for hydrogen storage applications, with properties similar to ZrNiH and HfNiH. This implies that structure mainly determines properties of all investigated hydrides in this class of intermetallics.

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E 7

HYDROGEN STORAGE, MICROSTRUCTURE AND MECHANICAL PROPERTIES OF $Mg_{65}Ni_{20}Cu_5Y_{10}$ METALLIC GLASS DEFORMED BY HIGH-PRESSURE TORSION

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Rapidly quenched amorphous $Mg_{65}Ni_{20}Cu_5Y_{10}$ metallic glass compacts were subjected to heavy shear deformation by high pressure torsion until different amount of ultimate strain. High resolution X-ray diffraction analysis and scanning electron microscopy revealed that high-pressure torsion resulted in a deformation dependent microstructure. Nanoindentation measurements indicated that the heavy shear deformation yields an increase in hardness. High-pressure calorimetry measurements revealed that hydrogen uptake in the fully amorphous alloy occurs at a significantly lower temperature compared to the fully crystallized state, while the amount of absorbed hydrogen increased considerably after heavy shear deformation due to the formation of Mg_2Ni crystals.

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E 8

EFFECTS OF PARTICLE SIZE AND TYPE OF CONDUCTIVE ADDITIVE ON THE ELECTRODE PERFORMANCES OF GAS ATOMIZED AB_5-TYPE HYDROGEN STORAGE ALLOY

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The structure, phase composition, surface condition of gas atomized powders of $LaNi_{4.5}Al_{0.5}$ depending on the particle size (fractions: ≤ 50 μm; 160-316 μm; 630-1000 μm) have been studied. The electrochemical and storage properties of electrodes made from these powders with the addition of conductive additives as electrolytic copper powder or composite carbon additive (1 wt.% nanotubes + 7 wt.% nanosized carbon black) have been examined. In this study were used such methods as XRD, SEM, RPS, EIS and several electrochemical methods. The results showed that gas atomized powders with larger particle size in the initial state show better kinetics of hydrogen exchange reactions and high discharge capacity (up to 300 mA*h/g). The electrodes from powders of all fractions have good ability to high-rate discharge. The discharge process of electrodes, regardless of particle size and type of conductive additive is controlled by diffusion of hydrogen in the electrode. With increasing particle size of the alloy in the electrode diffusion coefficients of hydrogen increase from $6\text{-}8\times10^{-12}$ cm^2/s for small and medium fractions to 3.5×10^{-10} cm^2/s for large fraction respectively. For electrode from $LaNi_{4.5}Al_{0.5}$ with composite carbon additive diffusion coefficients of hydrogen during discharge, calculated from the data obtained by EIS are in good agreement with those obtained from cyclic current-voltage curves ($2\text{-}4\times10^{-9}$ cm^2/s).

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E 9

HYDROGEN DESORPTION PROPERTIES OF $MgH_2/LiAlH_4$ COMPOSITES

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Hydrogen storage properties of MgH_2-$LiAlH_4$ composite obtained by mechanical milling for different milling times and different weight percentage of $LiAlH_4$ have been investigated by temperature programmed desorption (TPD). The morphology of samples has been investigated by XRD and SEM analysis and correlated with desorption properties. MgH_2-$LiAlH_4$ composites show improved hydrogen desorption characteristics in comparison with the pure milled MgH_2. It has been shown that quick mechanical milling/mixing of MgH_2 with small amount of $LiAlH_4$ shifts two characteristic hydrogen desorption maxima to the lower temperatures. The kinetics of hydrogen desorption in composites is also improved.

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E 10

EVALUATION OF THE HYDROGEN EMBRITTLEMENT OF METALLIC MEMBRANES BY THE DISK TEST METHOD

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The safety of metallic structures or membranes used for hydrogen storage is strongly conditioned by the sensitivity of their materials to hydrogen. This sensitivity is studied by the disk pressure testing and the external hydrogen embrittlement index is defined as the ratio of rupture pressures under helium and hydrogen, pHe/pH_2. The technique used simulates well the working conditions of pressure vessels and allows the identification of different effects related to the parameters of the environment, loading and material. The obtained data contribute to a better understanding of the embrittlement phenomenon, leading to a safer selection of appropriate materials for applications under gaseous hydrogen.

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E 11

ELECTRONIC STRUCTURE AND CHARGE TOPOLOGY STUDY OF ALKALI HYDRIDES

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Electronic structure and Bader charge analysis calculation of alkali hydride series has been performed. Classification of charge topology structures of alkali hydrides within the broader frame of NaCl structures (along with alkali halides) has been established. Additionally, connection between charge topology and experimentally observed trends in macroscopic properties, such as B1-B2 phase transformation pressures, melting points, elastic properties etc., was considered.

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E 12

REACTIVELY DEPOSITED THIN FILMS OF MAGNESIUM NICKEL HYDRIDE

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Uniform magnesium nickel hydride thin film was synthesized on large area glass substrate by reactive sputtering. Electrical and optical properties have shown the material of semiconducting nature with band gap of 1.6eV for the amorphous as-deposited sample and 2.1eV for the annealed sample with crystal structure. XRD results followed these transformations. Performed Hall measurements have shown wide range of resistivity. TPD measurements confirm release of hydrogen and also the release of impurity gases.

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E 13

INVESTIGATION OF NUCLEATION PROCESS IN MgH_2 THIN FILMS

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In attempt to understand and improve the desorption process, the nucleation of MgH_2 thin films during desorption were followed by *in situ* optical microscopy coupled with MS. We have traced the changes during desorption process in both irradiated and non irradiated thin films. It has been noticed that the nuclei change shape depends on quantity of defects. In fact, in non irradiated samples we have observed spherical nuclei while in irradiatied sample the shape is irregular. Both films exhibit modification in optical properties during desorption. To explain this feature an ab initio numerical calculation were done.

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E 14

PREPARATION AND CHARACTERIZATION OF MgH_2-BASED COMPOSITE PELLETS

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Focusing the attention to the application of MgH_2-base composites inside tanks for hydrogen storage, studies were carried out with MgH_2-based pellets prepared with the addition of Nb_2O_5 or Fe and carbon based materials. The sorption kinetic of the pellets was studied revealing the material to have a similar kinetic with respect to the powder. X-Ray diffraction analysis (XRD) and Scanning Electron Microscopy (SEM) observations of the inner core of the pellets (cross-sections), before and after the cycling process, were performed. The effects of air exposure were also investigated.

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E 15

HYDROGEN-INDUCED DEFECTS IN THIN FILMS CHARACTERIZED BY VARIABLE ENERGY SLOW POSITRON ANNIHILATION SPECTROSCOPY

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Positron annihilation spectroscopy (PAS) is a non-destructive technique which enables to characterize open volume defects and open space in lattice which is available for hydrogen. Positron is a unique probe of inter-atomic regions, grain boundaries and pores. Positron in solid matter is confined at open volume defects and annihilation radiation carries information about local electronic structure of these defects. Variable energy slow positron annihilation spectroscopy (VEPAS) uses slow positron beam with tuneable energy. Since positron penetration depth increases with increasing positron kinetic energy VEPAS enables to perform depth resolved defect studies of solid materials. In this work VEPAS was employed for characterization of hydrogen-induced defects in thin films. Hydrogen loading causes a significant volume expansion, which is isotropic in free-standing bulk materials. Contrary to bulk samples, thin films are clamped to an elastically hard substrate which prevents in-plane expansion. As a consequence, hydrogen loaded thin film may expand only in the out-of-plane direction. Hence, hydrogen-induced expansion of thin films is strongly non-uniform and hydrogen loading of thin films introduces very high internal stresses (in the GPa range). Due to these reasons, behaviour of hydrogen loaded thin films differs substantially from that of corresponding bulk samples. Using VEPAS it was found that stresses introduced by hydrogen cause plastic deformation of thin films and introduce a high concentration of open volume defects.

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E 16

MAGNESIUM NANOPARTICLES AND NANODOTS: SYNTHESIS, STRUCTURE AND HYDROGEN SORPTION

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We report on the synthesis of magnesium (Mg) nanostructures by means of two different techniques: Mg nanoparticles were prepared by inert gas condensation in a He flow, while Mg nanodots were grown by molecular beam epitaxy on a MgO substrate coated by ultra-thin alumina masks. The structure and morphology were characterized by electron microscopy, atomic force microscopy, and X-ray diffraction. First experiments aimed at the determination of the thermodynamics of hydrogen sorption by means of optical methods showed a dramatic increase of the plateau pressure for hydrogen absorption in Mg nanoparticles.

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E 17

VANADIUM OXIDE AS HYDROGEN TECHNOLOGY MATERIAL

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Vanadium oxide has been well known for its catalytic activity, while its various nanostructures have been synthesized for years now. In spite of this, there have been relatively few studies of use of vanadium oxide as a catalytic material for hydrogen technologies. We present an investigation of use of very thin films of vanadium oxide, using different supports, for hydrogen technology, with a view of anticipating the behavior of synthesized vanadium oxide nanostructures and determining the factors essential to performance of these materials and ways to incorporate these into physical systems.

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E 18

POSSIBLE PATHS OF HYDROGEN DIFFUSION IN TIO_2 – ROLE OF THE SURFACE

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We have investigated the hydrogen interaction with surface of rutile TiO_2 using pseudopotential method implemented in *Abinit* code. The hydrogen diffusion behavior and thermodynamic properties were calculated by means of full relaxation of structure in every step of bulk diffusion. The results show the existence of potential barriers close to every atomic layer and the trend of lowering of barriers and overall system energy away from surface. This goes in favor of previously experimental findings of TiO_2 low surface H coverage and easy diffusion of hydrogen into TiO_2 bulk.

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E 19

DESORPTION PROPERTIES OF MgH_2 DESTABILIZED WITH $NaNH_2$ CATALYST

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To destabilize MgH_2 lattice structure and improve hydrogen desorption properties mechanical milling of $MgH_2$with low amount of$NaNH_2$ has been performed. Therefore, the amide is used as a catalyst. Pre-milling of MgH_2 has been performed followed with composite formation during 15, 30 and 60 minutes. Microstructure of samples has been characterized by XRD and SEM analysis and correlated to desorption properties examined using Hydrogen Sorption Analyser and DSC analysis. DSC analysis show that desorption temperature is shifted towards lower values and also pointed out the significance of milling duration. It has been demonstrated that desorption kinetics is significantly improved.

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E 20

MICROSTRUCTURE OF ULTRAFINE-GRAINED WE43+12wt% Zn MAGNESIUM ALLOY AFTER EQUAL CHANNEL ANGULAR PRESSING

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Mg-based alloys are considered to be one of the most promising candidates as hydrogen storage media. In this work, we investigated microstructure of complex WE43 magnesium alloy modified by the addition of 12wt% Zn. In order to refine microstructure, the alloy was subjected to equal channel angular pressing with back-pressure (ECAP-BP) at temperature of 473 K. Samples after 4 passes by Bc route were analysed using light microscopy, scanning electron microscopy (SEM) and transmission electron microscopy (TEM). TEM microstructural examination revealed MgZnY icosahedral quasicrystalline phase, Zn rich phase and various particles in Mg matrix. An average grain size of magnesium matrix was about 400 nm.

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E 21

SEVERE PLASTIC DEFORMATION OF Mg-Mn ALLOY AT ROOM TEMPERATURE

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Aim of this work is to obtain extremely refined Mg-Mn alloy with an excess of defects which can serve as traps for hydrogen. Mg-Mn binary alloy was processed by Equal Channel Angular Pressing (ECAP) with backpressure at room temperature (RT).The microstructure observed by electron back-scatter diffraction (EBSD) and transmission electron microscopy (TEM) revealed significant grain refinement with an average grain size ~0.5µm. Thermal stability was examined by dilatometry up to 480°C. The results show first structural instability at ~80°C during heating. For thorough characterization tensile tests at RT were also conducted after 3 and 4 passes by ECAP.

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E 22

ENHANCING THE HYDROGEN GRAPHENE INTERACTION BY METAL DECORATION

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Theoretical calculations of metal decorated graphene predict an attractive orbital interaction, the Kubas interaction, of molecular hydrogen to the metal centers. In this case a noticeably higher heat of adsorption for the bound hydrogen and hence a higher desorption temperature as compared to physisorbed hydrogen is expected. Molecular hydrogen bound to metal decorated graphene is an ideal model system to study the Kubas interaction in detail and promote the understanding of the underlying fundamental principles. Furthermore it is a promising candidate for a cheap, lightweight, intermediate temperature hydrogen storage material.

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E 23

THE POTENTIAL APPLICATION OF HYDROGEN IN DEVELOPING COUNTRIES

Rabah Arkam

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Given the promising hydrogen internal combustion engines, an energy system can then be offered as an alternative or complementary energy system. This potential is driven by three drivers: 1. CO2: The problem is to make all efforts to reduce emissions of greenhouse gases, particularly CO2. 2. Energy independence: Using hydrogen and improve their geopolitical situation. 3. The inevitable exhaustion of fossil resources, we want to keep as a raw material (plastic ...) rather than burn them. Chemical, hydrogen energy, It is produced by reforming natural gas by electrolysis or thermo chemical relying on nuclear energy or renewable.

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